|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **Name** | **Molecular Formula** | **Structure** | **IUPAC International Chemical Identifier** |
|  | H | H |  | InChI=1S/H |
|  | H2 | H2 |  | InChI=1S/H2/h1H |
|  | O | O |  | InChI=1S/O |
|  | O2 | O2 |  | InChI=1S/O2/c1-2 |
|  | OH | OH |  | InChI=1S/HO/h1 |
|  | H2O | H2O |  | InChI=1S/H2O/h1H |
|  | H2O2 | H2O2 |  | InChI=1S/H2O2/c1-2/h1-2H |
|  | Ar | Ar |  | InChI=1S/Ar |
|  | CO | CO |  | InChI=1S/CO2/c2-1-3 |
|  | CO2 | CO2 |  | InChI=1S/CO2/c2-1-3 |
|  | CH2O | CH2O |  | InChI=1S/CH2O/c1-2/h1H2 |
|  | HCO | CHO |  | InChI=1S/CHO/c1-2/h1H |
|  | HO2CHO | CH2O3 |  | InChI=1S/CH2O3/c2-1-4-3/h1,3H |
|  | HCOH | CH2O |  | InChI=1S/CH2O/c1-2/h1-2H |
|  | O2CHO | CHO3 |  | InChI=1S/CHO3/c2-1-4-3/h1H |
|  | HOCHO | CH2O2 |  | InChI=1S/CH2O2/c2-1-3/h1H,(H,2,3) |
|  | OCHO | CHO2 |  | InChI=1S/CHO2/c2-1-3/h1H |
|  | HOCH2O2H | CH4O3 |  | InChI=1S/CH4O3/c2-1-4-3/h2-3H,1H2 |
|  | HOCH2O2 | CH3O3 |  | InChI=1S/CH3O3/c2-1-4-3/h2H,1H2 |
|  | OCH2O2H | CH3O3 |  | InChI=1S/CH3O3/c2-1-4-3/h3H,1H2 |
|  | HOCH2O | CH3O2 |  | InChI=1S/CH3O2/c2-1-3/h2H,1H2 |
|  | CH3OH | CH4O |  | InChI=1S/CH4O/c1-2/h2H,1H3 |
|  | CH2OH | CH3O |  | InChI=1S/CH3O/c1-2/h2H,1H2 |
|  | CH3O | CH3O |  | InChI=1S/CH3O/c1-2/h1H3 |
|  | CH3O2H | CH4O2 |  | InChI=1S/CH4O2/c1-3-2/h2H,1H3 |
|  | CH3O2 | CH3O2 |  | InChI=1S/CH3O2/c1-3-2/h1H3 |
|  | CH4 | CH4 |  | InChI=1S/CH4/h1H4 |
|  | CH3 | CH3 |  | InChI=1S/CH3/h1H3 |
|  | CH2 | CH2 |  | InChI=1S/CH2/h1H2 |
|  | C2H6 | C2H6 |  | InChI=1S/C2H6/c1-2/h1-2H3 |
|  | C2H5 | C2H5 |  | InChI=1S/C2H5/c1-2/h1H2,2H3 |
|  | C2H4 | C2H4 |  | InChI=1S/C2H4/c1-2/h1-2H2 |
|  | C2H3 | C2H3 |  | InChI=1S/C2H3/c1-2/h1H,2H2 |
|  | C2H2 | C2H2 |  | InChI=1S/C2H2/c1-2/h1-2H |
|  | C2H | C2H |  | InChI=1S/C2H/c1-2/h1H |
|  | CH3CHO | C2H4O |  | InChI=1S/C2H4O/c1-2-3/h2H,1H3 |
|  | C2H3OH | C2H4O |  | InChI=1S/C2H4O/c1-2-3/h2-3H,1H2 |
|  | C2H2OH | C2H3O |  | InChI=1S/C2H3O/c1-2-3/h1-3H |
|  | CH3CO | C2H3O |  | InChI=1S/C2H3O/c1-2-3/h1H3 |
|  | CH2CHO | C2H3O |  | InChI=1S/C2H3O/c1-2-3/h2H,1H2 |
|  | O2CH2CHO | C2H3O3 |  | InChI=1S/C2H3O3/c3-1-2-5-4/h1H,2H2 |
|  | HO2CH2CO | C2H3O3 |  | InChI=1S/C2H3O3/c3-1-2-5-4/h4H,2H2 |
|  | CH2CO | C2H2O |  | InChI=1S/C2H2O/c1-2-3/h1H2 |
|  | HCCO | C2HO |  | InChI=1S/C2HO/c1-2-3/h1H |
|  | HCCOH | C2H2O |  | InChI=1S/C2H2O/c1-2-3/h1,3H |
|  | CH3CO3H | C2H4O3 |  | InChI=1S/C2H4O3/c1-2(3)5-4/h4H,1H3 |
|  | CH3CO3 | C2H3O3 |  | InChI=1S/C2H3O3/c1-2(3)5-4/h1H3 |
|  | CH3CO2 | C2H3O2 |  | InChI=1S/C2H3O2/c1-2(3)4/h1H3 |
|  | C2H5OH | C2H6O |  | InChI=1S/C2H6O/c1-2-3/h3H,2H2,1H3 |
|  | C2H5O | C2H5O |  | InChI=1S/3C2H5O/c3\*1-2-3/h2H2,1H3;2-3H,1H3;3H,1-2H2 |
|  | sC2H4OH | C2H5O |  | InChI=1S/C2H5O/c1-2-3/h2-3H,1H3 |
|  | pC2H4OH | C2H5O |  | InChI=1S/C2H5O/c1-2-3/h3H,1-2H2 |
|  | O2C2H4O2 | C2H5O3 |  | InChI=1S/C2H5O3/c3-1-2-5-4/h3H,1-2H2 |
|  | C2H5O2H | C2H6O2 |  | InChI=1S/C2H6O2/c1-2-4-3/h3H,2H2,1H3 |
|  | C2H5O2 | C2H5O2 |  | InChI=1S/C2H5O2/c1-2-4-3/h2H2,1H3 |
|  | C2H4O2H | C2H5O2 |  | InChI=1S/C2H5O2/c1-2-4-3/h3H,1-2H2 |
|  | C2H4O1-2 | C2H4O |  | InChI=1S/C2H4O/c1-2-3-1/h1-2H2 |
|  | C2H3O1-2 | C2H3O |  | InChI=1S/C2H3O/c1-2-3-1/h1H,2H2 |
|  | CH3COCH3 | C3H6O |  | InChI=1S/C3H6O/c1-3(2)4/h1-2H3 |
|  | CH3COCH2 | C3H5O |  | InChI=1S/C3H5O/c1-3(2)4/h1H2,2H3 |
|  | CH3COCH2O2 | C3H5O3 |  | InChI=1S/C3H5O3/c1-3(4)2-6-5/h2H2,1H3 |
|  | C3KET21 | C3H6O3 |  | InChI=1S/C3H6O3/c1-3(4)2-6-5/h5H,2H2,1H3 |
|  | C2H3CHO | C3H4O |  | InChI=1S/C3H4O/c1-2-3-4/h2-3H,1H2 |
|  | C2H3CO | C3H3O |  | InChI=1S/C3H3O/c1-2-3-4/h2H,1H2 |
|  | C2H5CHO | C3H6O |  | InChI=1S/C3H6O/c1-2-3-4/h3H,2H2,1H3 |
|  | C2H5CO | C3H5O |  | InChI=1S/C3H5O/c1-2-3-4/h2H2,1H3 |
|  | CH3OCH3 | C2H6O |  | InChI=1S/C2H6O/c1-3-2/h1-2H3 |
|  | CH3OCH2 | C2H5O |  | InChI=1S/C2H5O/c1-3-2/h1H2,2H3 |
|  | CH3OCH2O2 | C2H5O3 |  | InChI=1S/C2H5O3/c1-4-2-5-3/h2H2,1H3 |
|  | CH2OCH2O2H | C2H5O3 |  | InChI=1S/C2H5O3/c1-4-2-5-3/h3H,1-2H2 |
|  | CH3OCH2O2H | C2H6O3 |  | InChI=1S/C2H6O3/c1-4-2-5-3/h3H,2H2,1H3 |
|  | CH3OCH2O | C2H5O2 |  | InChI=1S/C2H5O2/c1-4-2-3/h2H2,1H3 |
|  | O2CH2OCH2O2H | C2H5O5 |  | InChI=1S/C2H5O5/c3-6-1-5-2-7-4/h3H,1-2H2 |
|  | HO2CH2OCHO | C2H4O4 |  | InChI=1S/C2H4O4/c3-1-5-2-6-4/h1,4H,2H2 |
|  | OCH2OCHO | C2H3O3 |  | InChI=1S/C2H3O3/c3-1-5-2-4/h1H,2H2 |
|  | HOCH2OCO | C2H3O3 |  | InChI=1S/C2H3O3/c3-1-5-2-4/h3H,1H2 |
|  | CH3OCHO | C2H4O2 |  | InChI=1S/C2H4O2/c1-4-2-3/h2H,1H3 |
|  | CH3OCO | C2H3O2 |  | InChI=1S/C2H3O2/c1-4-2-3/h1H3 |
|  | CH2OCHO | C2H3O2 |  | InChI=1S/C2H3O2/c1-4-2-3/h2H,1H2 |
|  | He | He |  | InChI=1S/He |
|  | C3H8 | C3H8 |  | InChI=1S/C3H8/c1-3-2/h3H2,1-2H3 |
|  | iC3H7 | C3H7 |  | InChI=1S/C3H7/c1-3-2/h3H,1-2H3 |
|  | nC3H7 | C3H7 |  | InChI=1S/C3H7/c1-3-2/h1,3H2,2H3 |
|  | C3H6 | C3H6 |  | InChI=1S/C3H6/c1-3-2/h3H,1H2,2H3 |
|  | C3H5-A | C3H5 |  | InChI=1S/C3H5/c1-3-2/h3H,1-2H2 |
|  | C3H5-S | C3H5 |  | InChI=1S/C3H5/c1-3-2/h1,3H,2H3 |
|  | C3H5-T | C3H5 |  | InChI=1S/C3H5/c1-3-2/h1H2,2H3 |
|  | C3H4-P | C3H4 |  | InChI=1S/C3H4/c1-3-2/h1H,2H3 |
|  | C3H4-A | C3H4 |  | InChI=1S/C3H4/c1-3-2/h1-2H2 |
|  | C3H3 | C3H3 |  | InChI=1S/C3H3/c1-3-2/h1H,2H2 |
|  | C3H5O | C3H5O |  | InChI=1S/C3H5O/c1-2-3-4/h2H,1,3H2 |
|  | C3H6OOH1-2 | C3H7O2 |  | InChI=1S/C3H7O2/c1-2-3-5-4/h3-4H,2H2,1H3 |
|  | C3H6OOH1-3 | C3H7O2 |  | InChI=1S/C3H7O2/c1-2-3-5-4/h4H,1-3H2 |
|  | C3H6OOH2-1 | C3H7O2 |  | InChI=1S/C3H7O2/c1-3(2)5-4/h3-4H,1H2,2H3 |
|  | C3H6OOH1-2O2 | C3H7O4 |  | InChI=1S/C3H7O4/c1-2-3(6-4)7-5/h3-4H,2H2,1H3 |
|  | C3H6OOH1-3O2 | C3H7O4 |  | InChI=1S/C3H7O4/c4-6-2-1-3-7-5/h4H,1-3H2 |
|  | C3H6OOH2-1O2 | C3H7O4 |  | InChI=1S/C3H7O4/c1-3(7-5)2-6-4/h3,5H,2H2,1H3 |
|  | C3H6OOH2-2 | C3H7O2 |  | InChI=1S/C3H7O2/c1-3(2)5-4/h4H,1-2H3 |
|  | NC3H7O2H | C3H8O2 |  | InChI=1S/C3H8O2/c1-2-3-5-4/h4H,2-3H2,1H3 |
|  | IC3H7O2H | C3H8O2 |  | InChI=1S/C3H8O2/c1-3(2)5-4/h3-4H,1-2H3 |
|  | NC3H7O2 | C3H7O2 |  | InChI=1S/C3H7O2/c1-2-3-5-4/h2-3H2,1H3 |
|  | IC3H7O2 | C3H7O2 |  | InChI=1S/C3H7O2/c1-3(2)5-4/h3H,1-2H3 |
|  | NC3H7O | C3H7O |  | InChI=1S/C3H7O/c1-2-3-4/h2-3H2,1H3 |
|  | IC3H7O | C3H7O |  | InChI=1S/C3H7O/c1-3(2)4/h3H,1-2H3 |
|  | C3H6O1-2 | C3H6O |  | InChI=1S/C3H6O/c1-3-2-4-3/h3H,2H2,1H3 |
|  | C3H6O1-3 | C3H6O |  | InChI=1S/C3H6O/c1-2-4-3-1/h1-3H2 |
|  | C3KET12 | C3H6O3 |  | InChI=1S/C3H6O3/c1-3(2-4)6-5/h2-3,5H,1H3 |
|  | C3KET13 | C3H6O3 |  | InChI=1S/C3H6O3/c4-2-1-3-6-5/h2,5H,1,3H2 |
|  | C3H51-2,3OOH | C3H7O4 |  | InChI=1S/C3H7O4/c1-3(7-5)2-6-4/h3-5H,1-2H2 |
|  | C3H52-1,3OOH | C3H7O4 |  | InChI=1S/C3H7O4/c4-6-2-1-3-7-5/h1,4-5H,2-3H2 |
|  | C3H6OH | C3H7O |  | InChI=1S/C3H7O/c1-2-3-4/h2,4H,3H2,1H3 |
|  | HOC3H6O2 | C3H7O3 |  | InChI=1S/C3H7O3/c1-3(2-4)6-5/h3-4H,2H2,1H3 |
|  | CH3CHCO | C3H4O |  | InChI=1S/C3H4O/c1-2-3-4/h2H,1H3 |
|  | AC3H5OOH | C3H6O2 |  | InChI=1S/C3H6O2/c1-2-3-5-4/h2,4H,1,3H2 |
|  | C2H3OCH2 | C3H5O |  | InChI=1S/C4H7O/c1-3-4-5-2/h3H,1-2,4H2 |
|  | C2H3OOH | C2H4O2 |  | InChI=1S/C2H4O2/c1-2-4-3/h2-3H,1H2 |
|  | CC3H4 | C3H4 |  | InChI=1S/C3H4/c1-2-3-1/h1-2H,3H2 |
|  | H2CC | C2H2 |  | InChI=1S/C2H2/c1-2/h1H2 |
|  | C4H10 | C4H10 |  | InChI=1S/C4H10/c1-3-4-2/h3-4H2,1-2H3 |
|  | C4H8-1 | C4H8 |  | InChI=1S/C4H8/c1-3-4-2/h3H,1,4H2,2H3 |
|  | C4H8-2 | C4H8 |  | InChI=1S/C4H8/c1-3-4-2/h3-4H,1-2H3/b4-3+ |
|  | PC4H9 | C4H9 |  | InChI=1S/C4H9/c1-3-4-2/h1,3-4H2,2H3 |
|  | SC4H9 | C4H9 |  | InChI=1S/C4H9/c1-3-4-2/h3H,4H2,1-2H3 |
|  | C4H71-1 | C4H7 |  | InChI=1S/C4H7/c1-3-4-2/h1,3H,4H2,2H3 |
|  | C4H71-2 | C4H7 |  | InChI=1S/C4H7/c1-3-4-2/h1,4H2,2H3 |
|  | C4H71-3 | C4H7 |  | InChI=1S/C4H7/c1-3-4-2/h3-4H,1H2,2H3 |
|  | C4H71-4 | C4H7 |  | InChI=1S/C4H7/c1-3-4-2/h3H,1-2,4H2 |
|  | C4H72-2 | C4H7 |  | InChI=1S/C4H7/c1-3-4-2/h3H,1-2H3 |
|  | C4H6 | C4H6 |  | InChI=1S/C4H6/c1-3-4-2/h3-4H,1-2H2 |
|  | PC4H9O2H | C4H10O2 |  | InChI=1S/C4H10O2/c1-2-3-4-6-5/h5H,2-4H2,1H3 |
|  | SC4H9O2H | C4H10O2 |  | InChI=1S/C4H10O2/c1-3-4(2)6-5/h4-5H,3H2,1-2H3 |
|  | PC4H9O2 | C4H9O2 |  | InChI=1S/C4H9O2/c1-2-3-4-6-5/h2-4H2,1H3 |
|  | SC4H9O2 | C4H9O2 | z | InChI=1S/C4H9O2/c1-3-4(2)6-5/h4H,3H2,1-2H3 |
|  | PC4H9O | C4H9O |  | InChI=1S/C4H9O/c1-2-3-4-5/h2-4H2,1H3 |
|  | SC4H9O | C4H9O |  | InChI=1S/C4H9O/c1-3-4(2)5/h4H,3H2,1-2H3 |
|  | C4H7O | C4H7O |  | InChI=1S/C4H7O/c1-3-4(2)5/h3-4H,1H2,2H3 |
|  | C4H8O1-2 | C4H8O |  | InChI=1S/C4H8O/c1-2-4-3-5-4/h4H,2-3H2,1H3 |
|  | C4H8O1-3 | C4H8O |  | InChI=1S/C4H8O/c1-4-2-3-5-4/h4H,2-3H2,1H3 |
|  | C4H8O1-4 | C4H8O |  | InChI=1S/C4H8O/c1-2-4-5-3-1/h1-4H2 |
|  | C4H8O2-3 | C4H8O |  | InChI=1S/C4H8O/c1-3-4(2)5-3/h3-4H,1-2H3 |
|  | PC4H8OH | C4H9O |  | InChI=1S/C4H9O/c1-2-3-4-5/h3,5H,2,4H2,1H3 |
|  | SC4H8OH | C4H9O |  | InChI=1S/C4H9O/c1-3-4(2)5/h3-5H,1-2H3 |
|  | C4H8OH-1O2 | C4H9O3 |  | InChI=1S/C4H9O3/c1-2-3-4(5)7-6/h4-5H,2-3H2,1H3 |
|  | C4H8OH-2O2 | C4H9O3 |  | InChI=1S/C4H9O3/c1-3(5)4(2)7-6/h3-5H,1-2H3 |
|  | C4H8OOH1-1 | C4H9O2 |  | InChI=1S/C4H9O2/c1-2-3-4-6-5/h4-5H,2-3H2,1H3 |
|  | C4H8OOH1-2 | C4H9O2 |  | InChI=1S/C4H9O2/c1-2-3-4-6-5/h3,5H,2,4H2,1H3 |
|  | C4H8OOH1-3 | C4H9O2 |  | InChI=1S/C4H9O2/c1-2-3-4-6-5/h2,5H,3-4H2,1H3 |
|  | C4H8OOH1-4 | C4H9O2 |  | InChI=1S/C4H9O2/c1-2-3-4-6-5/h5H,1-4H2 |
|  | C4H8OOH2-1 | C4H9O2 |  | InChI=1S/C4H9O2/c1-3-4(2)6-5/h4-5H,2-3H2,1H3 |
|  | C4H8OOH2-2 | C4H9O2 |  | InChI=1S/C4H9O2/c1-3-4(2)6-5/h5H,3H2,1-2H3 |
|  | C4H8OOH2-3 | C4H9O2 |  | InChI=1S/C4H9O2/c1-3-4(2)6-5/h3-5H,1-2H3 |
|  | C4H8OOH2-4 | C4H9O2 |  | InChI=1S/C4H9O2/c1-3-4(2)6-5/h4-5H,1,3H2,2H3 |
|  | C4H8OOH1-2O2 | C4H9O4 |  | InChI=1S/C4H9O4/c1-2-4(8-6)3-7-5/h4-5H,2-3H2,1H3 |
|  | C4H8OOH1-3O2 | C4H9O4 |  | InChI=1S/C4H9O4/c1-4(8-6)2-3-7-5/h4-5H,2-3H2,1H3 |
|  | C4H8OOH1-4O2 | C4H9O4 |  | InChI=1S/C4H9O4/c5-7-3-1-2-4-8-6/h5H,1-4H2 |
|  | C4H8OOH2-1O2 | C4H9O4 |  | InChI=1S/C4H9O4/c1-2-4(8-6)3-7-5/h4,6H,2-3H2,1H3 |
|  | C4H8OOH2-3O2 | C4H9O4 |  | InChI=1S/C4H9O4/c1-3(7-5)4(2)8-6/h3-5H,1-2H3 |
|  | C4H8OOH2-4O2 | C4H9O4 |  | InChI=1S/C4H9O4/c1-4(8-6)2-3-7-5/h4,6H,2-3H2,1H3 |
|  | NC4KET12 | C4H8O3 |  | InChI=1S/C4H8O3/c1-2-4(3-5)7-6/h3-4,6H,2H2,1H3 |
|  | NC4KET13 | C4H8O3 |  | InChI=1S/C4H8O3/c1-4(7-6)2-3-5/h3-4,6H,2H2,1H3 |
|  | NC4KET14 | C4H8O3 |  | InChI=1S/C4H8O3/c5-3-1-2-4-7-6/h3,6H,1-2,4H2 |
|  | NC4KET21 | C4H8O3 |  | InChI=1S/C4H8O2/c1-2-3-4-6-5/h2-3,5H,4H2,1H3/b3-2+ |
|  | NC4KET23 | C4H8O3 |  | InChI=1S/C4H8O2/c1-3-4(2)6-5/h3,5H,1-2H3/b4-3+ |
|  | NC4KET24 | C4H8O3 |  | InChI=1S/C4H8O2/c1-2-3-4-6-5/h2-3,5H,4H2,1H3/b3-2- |
|  | C2H5COCH3 | C4H8O |  | InChI=1S/C4H8O/c1-3-4(2)5/h3H2,1-2H3 |
|  | C2H5COCH2 | C4H7O |  | InChI=1S/C4H7O/c1-3-4(2)5/h2-3H2,1H3 |
|  | CH2CH2COCH3 | C4H7O |  | InChI=1S/C4H7O/c1-3-4(2)5/h1,3H2,2H3 |
|  | CH3CHCOCH3 | C4H7O |  | InChI=1S/C4H7O/c1-3-4(2)5/h3H,1-2H3 |
|  | C2H3COCH3 | C4H6O |  | InChI=1S/C4H6O/c1-3-4(2)5/h3H,1H2,2H3 |
|  | CH3CHOOCOCH3 | C4H7O3 |  | InChI=1S/C4H7O3/c1-3(5)4(2)7-6/h4H,1-2H3 |
|  | CH2CHOOHCOCH3 | C4H7O3 |  | InChI=1S/C4H7O3/c1-3(5)4(2)7-6/h4,6H,2H2,1H3 |
|  | NC3H7CHO | C4H7O |  | InChI=1S/C4H8O/c1-2-3-4-5/h4H,2-3H2,1H3 |
|  | NC3H7CO | C4H7O |  | InChI=1S/C4H7O/c1-2-3-4-5/h2-3H2,1H3 |
|  | C3H6CHO-1 | C4H7O |  | InChI=1S/C4H7O/c1-2-3-4-5/h4H,1-3H2 |
|  | C3H6CHO-2 | C4H7O |  | InChI=1S/C4H7O/c1-2-3-4-5/h2,4H,3H2,1H3 |
|  | C3H6CHO-3 | C4H7O |  | InChI=1S/C4H7O/c1-2-3-4-5/h3-4H,2H2,1H3 |
|  | C2H5CHCO | C4H6O |  | InChI=1S/C4H6O/c1-2-3-4-5/h3H,2H2,1H3 |
|  | SC3H5CHO / CH3CHCHCHO | C4H6O |  | InChI=1S/C4H6O/c1-2-3-4-5/h2-4H,1H3/b3-2+ |
|  | SC3H5CO / CH3CHCHCO | C4H5O |  | InChI=1S/C4H5O/c1-2-3-4-5/h2-3H,1H3 |
|  | CH2CH2CHO | C3H5O |  | InChI=1S/C3H5O/c1-2-3-4/h3H,1-2H2 |
|  | IC4H10 | C4H10 |  | InChI=1S/C4H10/c1-4(2)3/h4H,1-3H3 |
|  | IC4H9 | C4H9 |  | InChI=1S/C4H9/c1-4(2)3/h4H,1H2,2-3H3 |
|  | TC4H9 | C4H9 |  | InChI=1S/C4H9/c1-4(2)3/h1-3H3 |
|  | IC4H8 | C4H8 |  | InChI=1S/C4H8/c1-4(2)3/h1H2,2-3H3 |
|  | IC4H7 | C4H7 |  | InChI=1S/C4H7/c1-4(2)3/h1-2H2,3H3 |
|  | TC4H9O2 | C4H9O2 |  | InChI=1S/C4H9O2/c1-4(2,3)6-5/h1-3H3 |
|  | IC4H9O2 | C4H9O2 |  | InChI=1S/C4H9O2/c1-4(2)3-6-5/h4H,3H2,1-2H3 |
|  | TC4H8O2H-I | C4H9O2 |  | InChI=1S/C4H9O2/c1-4(2,3)6-5/h5H,1H2,2-3H3 |
|  | IC4H8O2H-I | C4H9O2 |  | InChI=1S/C4H9O2/c1-4(2)3-6-5/h4-5H,1,3H2,2H3 |
|  | IC4H8O2H-T | C4H9O2 |  | InChI=1S/C4H9O2/c1-4(2)3-6-5/h5H,3H2,1-2H3 |
|  | IC4H8O | C4H8O |  | InChI=1S/C4H8O/c1-4(2)3-5-4/h3H2,1-2H3 |
|  | CC4H8O | C4H8O |  | InChI=1S/C4H8O/c1-4-2-3-5-4/h4H,2-3H2,1H3 |
|  | IC4H9O | C4H9O |  | InChI=1S/C4H9O/c1-4(2)3-5/h4H,3H2,1-2H3 |
|  | TC4H9O | C4H9O |  | InChI=1S/C4H9O/c1-4(2,3)5/h1-3H3 |
|  | IC4H9O2H | C4H10O2 |  | InChI=1S/C4H10O2/c1-4(2)3-6-5/h4-5H,3H2,1-2H3 |
|  | TC4H9O2H | C4H10O2 |  | InChI=1S/C4H10O2/c1-4(2,3)6-5/h5H,1-3H3 |
|  | IC4H7O | C4H7O |  | InChI=1S/C4H7O/c1-4(2)3-5/h1,3H2,2H3 |
|  | IC4H8OH | C4H9O |  | InChI=1S/C4H9O/c1-4(2)3-5/h4-5H,1,3H2,2H3 |
|  | IO2C4H8OH | C4H9O3 |  | InChI=1S/C4H9O3/c1-4(2-5)3-7-6/h4-5H,2-3H2,1H3 |
|  | IC3H7CHO | C4H8O |  | InChI=1S/C4H8O/c1-4(2)3-5/h3-4H,1-2H3 |
|  | TC3H6CHO | C4H7O |  | InChI=1S/C4H7O/c1-4(2)3-5/h3H,1-2H3 |
|  | IC3H7CO | C4H7O |  | InChI=1S/C4H7O/c1-4(2)3-5/h4H,1-2H3 |
|  | IC3H6CHO | C4H7O |  | InChI=1S/C4H7O/c1-4(2)3-5/h3-4H,1H2,2H3 |
|  | TC4H8OOH-IO2 | C4H9O4 |  | InChI=1S/C4H9O4/c1-4(2,8-6)3-7-5/h6H,3H2,1-2H3 |
|  | IC4H8OOH-IO2 | C4H9O4 |  | InChI=1S/C4H9O4/c1-4(2-7-5)3-8-6/h4-5H,2-3H2,1H3 |
|  | IC4H8OOH-TO2 | C4H9O4 |  | InChI=1S/C4H9O4/c1-4(2,8-6)3-7-5/h5H,3H2,1-2H3 |
|  | IC4KETII | C4H8O3 |  | InChI=1S/C4H8O3/c1-4(2-5)3-7-6/h2,4,6H,3H2,1H3 |
|  | IC4KETIT | C4H8O3 |  | InChI=1S/C4H8O3/c1-4(2,3-5)7-6/h3,6H,1-2H3 |
|  | IC4H7OH | C4H8O |  | InChI=1S/C4H8O/c1-4(2)3-5/h5H,1,3H2,2H3 |
|  | ICH4H6OH | C4H7O |  | InChI=1S/C4H7O/c1-4(2)3-5/h5H,1-3H2 |
|  | IC3H5CHO | C4H6O |  | InChI=1S/C4H6O/c1-4(2)3-5/h3H,1H2,2H3 |
|  | IC3H5CO | C4H5O |  | InChI=1S/C4H5O/c1-4(2)3-5/h1H2,2H3 |
|  | TC3H6OCHO | C4H7O2 |  | InChI=1S/C4H7O2/c1-4(2,6)3-5/h3H,1-2H3 |
|  | IC3H6CO | C4H7O |  | InChI=1S/C4H7O/c1-4(2)3-5/h4H,1-2H3 |
|  | IC4H7OOH | C4H8O2 |  | InChI=1S/C4H8O2/c1-4(2)3-6-5/h5H,1,3H2,2H3 |
|  | TC3H6OHCHO | C4H8O2 |  | InChI=1S/C4H8O2/c1-4(2,6)3-5/h3,6H,1-2H3 |
|  | TC3H6OH | C3H7O |  | InChI=1S/C3H7O/c1-3(2)4/h4H,1-2H3 |
|  | IC3H5OH | C3H6O |  | InChI=1S/C3H6O/c1-3(2)4/h4H,1H2,2H3 |
|  | SC3H5OH | C3H6O |  |  |
|  | TC3H6O2CHO | C4H7O3 |  | InChI=1S/C4H7O3/c1-4(2,3-5)7-6/h3H,1-2H3 |
|  | TC3H6O2HCO | C4H7O3 |  | InChI=1S/C4H7O3/c1-4(2,3-5)7-6/h6H,1-2H3 |
|  | IC3H5O2HCHO | C4H7O3 |  | InChI=1S/C4H7O3/c1-4(2,3-5)7-6/h3,6H,1H2,2H3 |
|  | CH2CCH2OH | C3H5O |  | InChI=1S/C3H5O/c1-2-3-4/h4H,1,3H2 |
|  | TC4H8CHO | C5H9O |  | InChI=1S/C5H9O/c1-5(2)3-4-6/h4H,3H2,1-2H3 |
|  | O2C4H8CHO | C5H9O3 |  | InChI=1S/C5H9O3/c1-5(2,8-7)3-4-6/h4H,3H2,1-2H3 |
|  | O2HC4H8CO | C5H9O3 |  | InChI=1S/C5H9O3/c1-5(2,8-7)3-4-6/h7H,3H2,1-2H3 |
|  | C3H5OH | C3H6O |  | InChI=1S/C3H6O/c1-2-3-4/h2,4H,1,3H2 |
|  | TIC4H7Q2-I | C4H9O4 |  | InChI=1S/C4H9O4/c1-4(2,8-6)3-7-5/h5-6H,1,3H2,2H3 |
|  | IIC4H7Q2-T | C4H9O4 |  | InChI=1S/C4H9O4/c1-4(2-7-5)3-8-6/h5-6H,2-3H2,1H3 |
|  | IIC4H7Q2-I | C4H9O4 |  | InChI=1S/C4H9O4/c1-4(2-7-5)3-8-6/h4-6H,1-3H2 |
|  | CH2O2H | CH3O2 |  | InChI=1S/CH3O2/c1-3-2/h2H,1H2 |
|  | C4H4 | C4H4 |  | InChI=1S/C4H4/c1-3-4-2/h1,4H,2H2 |
|  | C4H3-I | C4H3 |  | InChI=1S/C4H3/c1-3-4-2/h1H,2H2 |
|  | C4H3-N | C4H3 |  | InChI=1S/C4H3/c1-3-4-2/h1-3H |
|  | C4H612 | C4H6 |  | InChI=1S/C4H6/c1-3-4-2/h4H,1H2,2H3 |
|  | C4H2 | C4H2 |  | InChI=1S/C4H2/c1-3-4-2/h1-2H |
|  | C4H5-I | C4H5 |  | InChI=1S/C4H5/c1-3-4-2/h1H2,2H3 |
|  | C4H5-N | C4H5 |  | InChI=1S/C4H5/c1-3-4-2/h1,3-4H,2H2 |
|  | C4H6O25 |  |  |  |
|  | C2H3CHOCH2 | C4H5O |  | InChI=1S/C4H5O/c1-3-4(2)5/h3H,1-2H2 |
|  | C4H5-2 | C4H5 |  | InChI=1S/C4H5/c1-3-4-/h1H2,2H3 |
|  | C4H6-2 | C4H6 |  | InChI=1S/C4H6/c1-3-4-2/h1-2H3 |
|  | C4H6O23 |  |  |  |
|  | C4H4O | C4H4O |  | InChI=1S/C4H4O/c1-2-3-4-5/h4H,1H3 |
|  | H2C4O |  |  |  |
|  | SC3H4OH | C3H5O |  | InChI=1S/C3H5O/c1-3(2)4/h4H,1-2H2 |
|  | PC3H4OH-2 | C3H5O |  | InChI=1S/C3H5O/c1-2-3-4/h3-4H,1H3 |
|  | CH3CHCHO | C3H5O |  | InChI=1S/C3H4O/c1-2-3-4/h2H,1H3 |
|  | C6H10 | C6H10 |  | InChI=1S/C6H10/c1-3-5-6-4-2/h3-4H,1-2,5-6H2 |
|  | C6H9-a | C6H9 |  | InChI=1S/C6H10/c1-3-5-6-4-2/h3-4H,1-2,5-6H2 |
|  | aC4H7OOH | C4H78O2 |  | InChI=1S/C4H8O2/c1-3-4-6-5-2/h3H,1,4H2,2H3 |
|  | C3H3 | C3H3 |  | InChI=1S/C3H3/c1-3-2/h1H,2H2 |
|  | C3H3O2H | C3H4O2 |  | IInChI=1/C3H4O2/c1-2-3-5-4/h3-4H,1H2 |
|  | C3H3O2H | C3H4O2 |  | InChI=1S/C3H2O/c1-2-3-4/h1,3H |
|  | IC4H7-I1 | C4H7 |  | Therm calculated |
|  | IC3H5OCH3 | C4H8O |  | Multiwell\_thermo  calculated |
|  | IC3H5OCH2 | C4H7O |  | Multiwell\_thermo  calculated |
|  | IC4H9OH | C4H10O |  |  |
|  | IC4H8OH-IT | C4H9O |  |  |
|  | TC4H9OH | C4H10O |  |  |
|  | IC4H8OH-TI | C4H9O |  |  |
|  | TQJC4H8OH | C4H9O3 |  |  |
|  | TQC4H8OI | C4H9O3 |  |  |
|  | TQC4H7OHI | C4H9O3 |  |  |
|  | QC4H7OHP | C4H9O3 |  |  |
|  | IQJC4H8OH | C4H9O3 |  |  |
|  | IQC4H8OT | C4H9O3 |  |  |
|  | IQC4H7OHT | C4H9O3 |  |  |
|  | C2CY(COC)OH | C4H8O2 |  |  |
|  | CCY(CCO)COH | C4H8O2 |  |  |
|  | CCY(CCOC)OH | C4H8O2 |  |  |
|  | SC4H7OH-I | C4H8O |  | Multiwell\_thermo  Calculated |
|  | SC4H7OH-IP | C4H7O |  | Multiwell\_thermo  Calculated |
|  | IC3H6OHCHO | C4H8O2 |  |  |
|  | CH3COCOOH | C3H6O3 |  |  |
|  | IC3H5COOH | C4H8O2 |  |  |
|  | IC3H5COHQ | C4H8O3 |  |  |
|  | IC3H5Q | C3H6O2 |  |  |
|  | TQC4H7OHIO2 | C4H9O5 |  |  |
|  | TQC4H7OHIQ-I | C4H9O5 |  |  |
|  | TQC4H7OHIQ-P | C4H9O5 |  |  |
|  | TQC4H7OHTO2 | C4H9O5 |  |  |
|  | HOCOCQ(CH3)2 | C4H8O4 |  |  |
|  | IQC4H7OHTO2 | C4H9O5 |  |  |
|  | IQC4H7OHTQ-P | C4H9O5 |  |  |
|  | IQC4H8OTQ-I | C4H9O5 |  |  |
|  | CH2COHCH2OOH | C3H6O3 |  |  |
|  | CH2COH | C2H3O |  |  |
|  | CH2C(CH2OOH)2 | C4H8O4 |  |  |
|  | CO(CH2OOH)2 | C3H6O5 |  |  |
|  | CHOC(CH3)OHCH2Q | C4H8O4 |  |  |
|  | CH3COCHO | C3H4O2 |  |  |
|  | COHQCYC(COC) | C4H8O4 |  |  |
|  | QCYC(CCOC)OH | C4H8O4 |  |  |
|  | IC4H7O2 | C4H7O2 |  |  |
|  | IC4H6OOH-I | C4H7O2 |  |  |
|  | C\*CYCCOC | C4h6o |  |  |
|  | CCYCCOOC-T1 | C4H7O2 |  |  |
|  | CCYCCOOC-I2 | C4H7O2 |  |  |
|  | CHOIC3H6O | C4H7O2 |  |  |
|  | CCY(C2O)CO | C4H7O2 |  |  |
|  | CCY(C2O)-T1 | C3H5O |  |  |
|  | C2CYCOOC-I1 | C4H7O2 |  |  |
|  | IC3H5OOCH2 | C4H7O2 |  |  |
|  | O2IC4H6OOH-I | C4H7O4 |  |  |
|  | H15de25dm | C8H14 |  |  |
|  | H15de25dm-S | C8H13 |  |  |
|  | H15de25dm-A | C8H13 |  |  |
|  | H15DE25DM-AO | C8H13O |  |  |
|  | H15DE25DM-SO | C8H13O |  |  |
|  | H15DE2M-T | C7H11 |  |  |
|  | IC4H7CHO | C5H8O |  |  |
|  | CCYCCC | C4H8 |  |  |
|  | B13DE2M | C5H8 |  |  |
|  | B13DE2MJ | C5H7 |  |  |
|  | AC5H9-D | C5H9 |  |  |
|  | AC5H9-C | C5H9 |  |  |
|  | CC5H9-A | C5H9 |  |  |
|  | AC5H9O-C | C5H9O |  |  |
|  | B2E2M1OJ | C5H9O |  |  |
|  | B1E3M3OJ | C5H9O |  |  |
|  | B2E3M1OJ | C5H9O |  |  |
|  | B12DE3M | C5H8 |  |  |
|  | IC3H4CHO-A | C4H5O |  |  |
|  | AC5H10 | C5H10 |  |  |
|  | AC5H9-A2 | C5H9 |  |  |
|  | NC5H12 | C5H12 |  |  |
|  | C5H11-1 | C5H11 |  |  |
|  | C5H11-2 | C5H11 |  |  |
|  | C5H11-3 | C5H11 |  |  |
|  | C5H10-1 | C5H10 |  |  |
|  | C5H10-2 | C5H10 |  |  |
|  | C5H91-3 | C5H9 |  |  |
|  | C5H91-4 | C5H9 |  |  |
|  | C5H91-5 | C5H9 |  |  |
|  | C5H92-4 | C5H9 |  |  |
|  | C5H92-5 | C5H9 |  |  |
|  | C5H81-3 | C5H8 |  |  |
|  | C5H9O1-3 | C5H9O |  |  |
|  | C5H9O2-4 | C5H9O |  |  |
|  | C5H11O-1 | C5H11O |  |  |
|  | C5H11O-2 | C5H11O |  |  |
|  | C5H11O-3 | C5H11O |  |  |
|  | C5H11O2-1 | C5H11O2 |  |  |
|  | C5H11O2-2 | C5H11O2 |  |  |
|  | C5H11O2-3 | C5H11O2 |  |  |
|  |  |  |  |  |
|  |  |  |  |  |