

Pentanedioic acid, 2-methyl-, dimethyl ester

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| Other names: | Glutaric acid, 2-methyl-, dimethyl ester «alpha»-Methylglutaric acid dimethyl ester Dimethyl «alpha»-methylglutarate Dimethyl 2-methylpentane-1,5-dioate Pentanedioic acid, 2-methyl-, 1,5-dimethyl ester Dimethyl-2-Methyl Glutarate |
| Inchi: | InChI=1S/C8H14O4/c1-6(8(10)12-3)4-5-7(9)11-2/h6H,4-5H2,1-3H3 |
| InchiKey: | ZWKRUNHAVNSFW-UHFFFAOYSA-N |
| Formula: | C8H14O4 |
| SMILES: | <chem>COC(=O)CCC(C)C(=O)OC</chem> |
| Mol. weight [g/mol]: | 174.19 |
| CAS: | 14035-94-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -453.80 | kJ/mol | Joback Method |
| hf | -703.33 | kJ/mol | Joback Method |
| hfus | 18.53 | kJ/mol | Joback Method |
| hvap | 51.33 | kJ/mol | Joback Method |
| log10ws | -0.65 | | Crippen Method |
| logp | 0.749 | | Crippen Method |
| mcvol | 138.460 | ml/mol | McGowan Method |
| pc | 2811.36 | kPa | Joback Method |
| tb | 534.58 | K | Joback Method |
| tc | 722.01 | K | Joback Method |
| tf | 309.24 | K | Joback Method |
| vc | 0.525 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 322.54 | J/mol×K | 534.58 | Joback Method |
| cpg | 376.76 | J/mol×K | 690.77 | Joback Method |
| cpg | 366.85 | J/mol×K | 659.53 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 356.46 | J/molxK | 628.29 | Joback Method |
| cpg | 345.61 | J/molxK | 597.06 | Joback Method |
| cpg | 334.30 | J/molxK | 565.82 | Joback Method |
| cpg | 386.20 | J/molxK | 722.01 | Joback Method |
| dvisc | 0.0002153 | Paxs | 534.58 | Joback Method |
| dvisc | 0.0002792 | Paxs | 497.02 | Joback Method |
| dvisc | 0.0003777 | Paxs | 459.47 | Joback Method |
| dvisc | 0.0005393 | Paxs | 421.91 | Joback Method |
| dvisc | 0.0008255 | Paxs | 384.35 | Joback Method |
| dvisc | 0.0013856 | Paxs | 346.80 | Joback Method |
| dvisc | 0.0026376 | Paxs | 309.24 | Joback Method |

Sources

| | |
|------------------------|---|
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C14035940&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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