

Glutaric acid, di(4,4-dimethylpent-2-yl) ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C19H36O4/c1-14(12-18(3,4)5)22-16(20)10-9-11-17(21)23-15(2)13-19(6,7)8/h1 |
| InchiKey: | IDPPTIXDECFRCY-UHFFFAOYSA-N |
| Formula: | C19H36O4 |
| SMILES: | CC(CC(C)(C)C)OC(=O)CCCC(=O)OC(C)CC(C)(C)C |
| Mol. weight [g/mol]: | 328.49 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -357.94 | kJ/mol | Joback Method |
| hf | -953.15 | kJ/mol | Joback Method |
| hfus | 28.67 | kJ/mol | Joback Method |
| hvap | 72.83 | kJ/mol | Joback Method |
| log10ws | -5.24 | | Crippen Method |
| logp | 4.893 | | Crippen Method |
| mvol | 293.450 | ml/mol | McGowan Method |
| pc | 1192.35 | kPa | Joback Method |
| rmpol | 2102.00 | | NIST Webbook |
| tb | 779.36 | K | Joback Method |
| tc | 971.10 | K | Joback Method |
| tf | 423.05 | K | Joback Method |
| vc | 1.113 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 912.49 | J/molxK | 779.36 | Joback Method |
| cpg | 993.96 | J/molxK | 939.15 | Joback Method |
| cpg | 979.69 | J/molxK | 907.19 | Joback Method |
| cpg | 964.46 | J/molxK | 875.23 | Joback Method |
| cpg | 948.21 | J/molxK | 843.27 | Joback Method |
| cpg | 930.90 | J/molxK | 811.32 | Joback Method |
| cpg | 1007.30 | J/molxK | 971.10 | Joback Method |
| dvisc | 0.0000341 | Paxs | 779.36 | Joback Method |
| dvisc | 0.0000489 | Paxs | 719.98 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000747 | Paxs | 660.59 | Joback Method |
| dvisc | 0.0001240 | Paxs | 601.20 | Joback Method |
| dvisc | 0.0002302 | Paxs | 541.82 | Joback Method |
| dvisc | 0.0004975 | Paxs | 482.43 | Joback Method |
| dvisc | 0.0013351 | Paxs | 423.05 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U377612&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

| | |
|-----------------|---|
| 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 |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/50-513-6/Glutaric-acid-di-4-4-dimethylpent-2-yl-ester.pdf>

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