

Glutaric acid, hexyl 6-methylhept-2-yl ester

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

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -363.62 | kJ/mol | Joback Method |
| hf | -935.65 | kJ/mol | Joback Method |
| hfus | 43.49 | kJ/mol | Joback Method |
| hvap | 75.42 | kJ/mol | Joback Method |
| log10ws | -5.37 | | Crippen Method |
| logp | 5.038 | | Crippen Method |
| mcvol | 293.450 | ml/mol | McGowan Method |
| pc | 1161.66 | kPa | Joback Method |
| rinpol | 2167.00 | | NIST Webbook |
| rinpol | 2167.00 | | NIST Webbook |
| tb | 785.82 | K | Joback Method |
| tc | 968.88 | K | Joback Method |
| tf | 418.21 | K | Joback Method |
| vc | 1.135 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 909.87 | J/molxK | 785.82 | Joback Method |
| cpg | 927.92 | J/molxK | 816.33 | Joback Method |
| cpg | 944.96 | J/molxK | 846.84 | Joback Method |
| cpg | 961.00 | J/molxK | 877.35 | Joback Method |
| cpg | 976.05 | J/molxK | 907.86 | Joback Method |
| cpg | 990.13 | J/molxK | 938.37 | Joback Method |
| cpg | 1003.26 | J/molxK | 968.88 | Joback Method |
| dvisc | 0.0013492 | Paxs | 418.21 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0005543 | Paxs | 479.48 | Joback Method |
| dvisc | 0.0002785 | Paxs | 540.75 | Joback Method |
| dvisc | 0.0001610 | Paxs | 602.01 | Joback Method |
| dvisc | 0.0001030 | Paxs | 663.28 | Joback Method |
| dvisc | 0.0000711 | Paxs | 724.55 | Joback Method |
| dvisc | 0.0000520 | Paxs | 785.82 | Joback Method |

Sources

| | |
|------------------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U377172&Units=SI |

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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