

Glutaric acid, cyclohexylmethyl 2-decyl ester

Inchi: InChI=1S/C22H40O4/c1-3-4-5-6-7-9-13-19(2)26-22(24)17-12-16-21(23)25-18-20-14-10-8
InchiKey: RMSSRGFEYAYWMW-UHFFFAOYSA-N
Formula: C22H40O4
SMILES: CCCCCCCC(C)OC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 368.55

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -311.47 | kJ/mol | Joback Method |
| hf | -937.97 | kJ/mol | Joback Method |
| hfus | 46.62 | kJ/mol | Joback Method |
| hvap | 82.92 | kJ/mol | Joback Method |
| log10ws | -6.52 | | Crippen Method |
| logp | 5.963 | | Crippen Method |
| mvol | 324.860 | ml/mol | McGowan Method |
| pc | 1092.82 | kPa | Joback Method |
| rinpol | 2527.00 | | NIST Webbook |
| rinpol | 2527.00 | | NIST Webbook |
| tb | 874.45 | K | Joback Method |
| tc | 1075.03 | K | Joback Method |
| tf | 474.40 | K | Joback Method |
| vc | 1.242 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1090.01 | J/molxK | 874.45 | Joback Method |
| cpg | 1172.25 | J/molxK | 1041.60 | Joback Method |
| cpg | 1158.53 | J/molxK | 1008.17 | Joback Method |
| cpg | 1143.48 | J/molxK | 974.74 | Joback Method |
| cpg | 1127.06 | J/molxK | 941.31 | Joback Method |
| cpg | 1109.25 | J/molxK | 907.88 | Joback Method |
| cpg | 1184.66 | J/molxK | 1075.03 | Joback Method |
| dvisc | 0.0000375 | Paxs | 874.45 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000511 | Paxs | 807.77 | Joback Method |
| dvisc | 0.0000736 | Paxs | 741.10 | Joback Method |
| dvisc | 0.0001140 | Paxs | 674.42 | Joback Method |
| dvisc | 0.0001944 | Paxs | 607.75 | Joback Method |
| dvisc | 0.0003781 | Paxs | 541.07 | Joback Method |
| dvisc | 0.0008866 | Paxs | 474.40 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U393510&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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