

Glutaric acid, 2,2-dichloroethyl 2-heptyl ester

Inchi: InChI=1S/C14H24Cl2O4/c1-3-4-5-7-11(2)20-14(18)9-6-8-13(17)19-10-12(15)16/h11-12H
InchiKey: LJFUXOZOYMEPGO-UHFFFAOYSA-N
Formula: C14H24Cl2O4
SMILES: CCCCCC(C)OC(=O)CCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 327.24

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -429.58 | kJ/mol | Joback Method |
| hf | -863.93 | kJ/mol | Joback Method |
| hfus | 38.94 | kJ/mol | Joback Method |
| hvap | 73.06 | kJ/mol | Joback Method |
| log10ws | -4.43 | | Crippen Method |
| logp | 4.016 | | Crippen Method |
| mcvol | 247.480 | ml/mol | McGowan Method |
| pc | 1564.75 | kPa | Joback Method |
| rinpol | 1965.00 | | NIST Webbook |
| rinpol | 1965.00 | | NIST Webbook |
| tb | 746.28 | K | Joback Method |
| tc | 936.02 | K | Joback Method |
| tf | 421.70 | K | Joback Method |
| vc | 0.954 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 682.41 | J/molxK | 746.28 | Joback Method |
| cpg | 696.76 | J/molxK | 777.90 | Joback Method |
| cpg | 710.26 | J/molxK | 809.53 | Joback Method |
| cpg | 722.93 | J/molxK | 841.15 | Joback Method |
| cpg | 734.78 | J/molxK | 872.77 | Joback Method |
| cpg | 745.80 | J/molxK | 904.40 | Joback Method |
| cpg | 756.02 | J/molxK | 936.02 | Joback Method |
| dvisc | 0.0014066 | Paxs | 421.70 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0006641 | Paxs | 475.80 | Joback Method |
| dvisc | 0.0003655 | Paxs | 529.89 | Joback Method |
| dvisc | 0.0002247 | Paxs | 583.99 | Joback Method |
| dvisc | 0.0001500 | Paxs | 638.09 | Joback Method |
| dvisc | 0.0001067 | Paxs | 692.18 | Joback Method |
| dvisc | 0.0000797 | Paxs | 746.28 | 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=U393582&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|----------------------------|---|
| cp_g: | 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: | Log ₁₀ of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| m_{cvol}: | 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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