

Glutaric acid, 2,4-dichlorobenzyl octyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C20H28Cl2O4/c1-2-3-4-5-6-7-13-25-19(23)9-8-10-20(24)26-15-16-11-12-17(2 |
| InchiKey: | PTOGRCKPIZQGT-UHFFFAOYSA-N |
| Formula: | C20H28Cl2O4 |
| SMILES: | CCCCCCCCOC(=O)CCCC(=O)OCc1ccc(Cl)cc1Cl |
| Mol. weight [g/mol]: | 403.34 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -281.03 | kJ/mol | Joback Method |
| hf | -763.62 | kJ/mol | Joback Method |
| hfus | 54.79 | kJ/mol | Joback Method |
| hvap | 90.80 | kJ/mol | Joback Method |
| log10ws | -6.89 | | Crippen Method |
| logp | 6.111 | | Crippen Method |
| mvol | 308.260 | ml/mol | McGowan Method |
| pc | 1258.37 | kPa | Joback Method |
| rinpol | 2825.00 | | NIST Webbook |
| tb | 921.08 | K | Joback Method |
| tc | 1133.06 | K | Joback Method |
| tf | 570.78 | K | Joback Method |
| vc | 1.194 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 929.13 | J/molxK | 921.08 | Joback Method |
| cpg | 942.84 | J/molxK | 956.41 | Joback Method |
| cpg | 955.36 | J/molxK | 991.74 | Joback Method |
| cpg | 966.72 | J/molxK | 1027.07 | Joback Method |
| cpg | 976.94 | J/molxK | 1062.40 | Joback Method |
| cpg | 986.04 | J/molxK | 1097.73 | Joback Method |
| cpg | 994.05 | J/molxK | 1133.06 | Joback Method |
| dvisc | 0.0003466 | Paxs | 570.78 | Joback Method |
| dvisc | 0.0002059 | Paxs | 629.16 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001336 | Paxs | 687.55 | Joback Method |
| dvisc | 0.0000928 | Paxs | 745.93 | Joback Method |
| dvisc | 0.0000679 | Paxs | 804.31 | Joback Method |
| dvisc | 0.0000519 | Paxs | 862.70 | Joback Method |
| dvisc | 0.0000410 | Paxs | 921.08 | 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=U376807&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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<https://www.chemeo.com/cid/36-669-0/Glutaric-acid-2-4-dichlorobenzyl-octyl-ester.pdf>

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