

Glutaric acid, 2,3-dichlorophenyl octyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C19H26Cl2O4/c1-2-3-4-5-6-7-14-24-17(22)12-9-13-18(23)25-16-11-8-10-15(20) |
| InchiKey: | ZLGXNZMSVQQSQI-UHFFFAOYSA-N |
| Formula: | C19H26Cl2O4 |
| SMILES: | CCCCCCCCOC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl |
| Mol. weight [g/mol]: | 389.31 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -289.45 | kJ/mol | Joback Method |
| hf | -742.98 | kJ/mol | Joback Method |
| hfus | 52.20 | kJ/mol | Joback Method |
| hvap | 88.57 | kJ/mol | Joback Method |
| log10ws | -6.62 | | Crippen Method |
| logp | 5.973 | | Crippen Method |
| mcvol | 294.170 | ml/mol | McGowan Method |
| pc | 1348.67 | kPa | Joback Method |
| rinpol | 2786.00 | | NIST Webbook |
| rinpol | 2786.00 | | NIST Webbook |
| tb | 898.20 | K | Joback Method |
| tc | 1108.62 | K | Joback Method |
| tf | 559.51 | K | Joback Method |
| vc | 1.137 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 870.45 | J/molxK | 898.20 | Joback Method |
| cpg | 926.82 | J/molxK | 1073.55 | Joback Method |
| cpg | 917.74 | J/molxK | 1038.48 | Joback Method |
| cpg | 907.58 | J/molxK | 1003.41 | Joback Method |
| cpg | 896.32 | J/molxK | 968.34 | Joback Method |
| cpg | 883.95 | J/molxK | 933.27 | Joback Method |
| cpg | 934.86 | J/molxK | 1108.62 | Joback Method |
| dvisc | 0.0000475 | Paxs | 898.20 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000599 | Paxs | 841.75 | Joback Method |
| dvisc | 0.0000781 | Paxs | 785.30 | Joback Method |
| dvisc | 0.0001062 | Paxs | 728.86 | Joback Method |
| dvisc | 0.0001519 | Paxs | 672.41 | Joback Method |
| dvisc | 0.0002321 | Paxs | 615.96 | Joback Method |
| dvisc | 0.0003863 | Paxs | 559.51 | 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=U359232&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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