

Glutaric acid, hept-2-yl 2,4-dichlorophenyl ester

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|----------------------|---|
| Inchi: | InChI=1S/C18H24Cl2O4/c1-3-4-5-7-13(2)23-17(21)8-6-9-18(22)24-16-11-10-14(19)12-15 |
| InchiKey: | UYKUTVYROUDLNM-UHFFFAOYSA-N |
| Formula: | C18H24Cl2O4 |
| SMILES: | CCCCC(C)OC(=O)CCCC(=O)Oc1ccc(Cl)cc1Cl |
| Mol. weight [g/mol]: | 375.29 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -300.31 | kJ/mol | Joback Method |
| hf | -727.62 | kJ/mol | Joback Method |
| hfus | 46.08 | kJ/mol | Joback Method |
| hvap | 85.96 | kJ/mol | Joback Method |
| log10ws | -6.32 | | Crippen Method |
| logp | 5.581 | | Crippen Method |
| mcvol | 280.080 | ml/mol | McGowan Method |
| pc | 1457.90 | kPa | Joback Method |
| rinpol | 2495.00 | | NIST Webbook |
| rinpol | 2495.00 | | NIST Webbook |
| tb | 874.88 | K | Joback Method |
| tc | 1086.47 | K | Joback Method |
| tf | 533.24 | K | Joback Method |
| vc | 1.075 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 813.01 | J/molxK | 874.88 | Joback Method |
| cpg | 826.39 | J/molxK | 910.15 | Joback Method |
| cpg | 838.66 | J/molxK | 945.41 | Joback Method |
| cpg | 849.82 | J/molxK | 980.68 | Joback Method |
| cpg | 859.90 | J/molxK | 1015.94 | Joback Method |
| cpg | 868.92 | J/molxK | 1051.21 | Joback Method |
| cpg | 876.88 | J/molxK | 1086.47 | Joback Method |
| dvisc | 0.0004701 | Paxs | 533.24 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0002706 | Paxs | 590.18 | Joback Method |
| dvisc | 0.0001716 | Paxs | 647.12 | Joback Method |
| dvisc | 0.0001172 | Paxs | 704.06 | Joback Method |
| dvisc | 0.0000847 | Paxs | 761.00 | Joback Method |
| dvisc | 0.0000641 | Paxs | 817.94 | Joback Method |
| dvisc | 0.0000503 | Paxs | 874.88 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U391852&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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