

Glutaric acid, 2,3-dichlorophenyl 2-ethylhexyl ester

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

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -291.89 | kJ/mol | Joback Method |
| hf | -748.26 | kJ/mol | Joback Method |
| hfus | 48.67 | kJ/mol | Joback Method |
| hvap | 88.18 | kJ/mol | Joback Method |
| log10ws | -6.38 | | Crippen Method |
| logp | 5.829 | | Crippen Method |
| mvol | 294.170 | ml/mol | McGowan Method |
| pc | 1356.63 | kPa | Joback Method |
| rinpol | 2664.00 | | NIST Webbook |
| rinpol | 2664.00 | | NIST Webbook |
| tb | 897.76 | K | Joback Method |
| tc | 1109.78 | K | Joback Method |
| tf | 544.51 | K | Joback Method |
| vc | 1.131 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 870.96 | J/molxK | 897.76 | Joback Method |
| cpg | 884.54 | J/molxK | 933.10 | Joback Method |
| cpg | 896.95 | J/molxK | 968.43 | Joback Method |
| cpg | 908.22 | J/molxK | 1003.77 | Joback Method |
| cpg | 918.36 | J/molxK | 1039.10 | Joback Method |
| cpg | 927.40 | J/molxK | 1074.44 | Joback Method |
| cpg | 935.37 | J/molxK | 1109.78 | Joback Method |
| dvisc | 0.0004221 | Paxs | 544.51 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0002401 | Paxs | 603.38 | Joback Method |
| dvisc | 0.0001510 | Paxs | 662.26 | Joback Method |
| dvisc | 0.0001025 | Paxs | 721.13 | Joback Method |
| dvisc | 0.0000737 | Paxs | 780.01 | Joback Method |
| dvisc | 0.0000555 | Paxs | 838.88 | Joback Method |
| dvisc | 0.0000434 | Paxs | 897.76 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U391474&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

Legend

| | |
|----------------------------|---|
| cp_g: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| g_f: | Standard Gibbs free energy of formation |
| h_f: | Enthalpy of formation at standard conditions |
| h_{fus}: | Enthalpy of fusion at standard conditions |
| h_{vap}: | Enthalpy of vaporization at standard conditions |
| log₁₀ws: | Log ₁₀ of Water solubility in mol/l |
| log_p: | 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 |

Latest version available from:

<https://www.chemeo.com/cid/121-328-3/Glutaric-acid-2-3-dichlorophenyl-2-ethylhexyl-ester.pdf>

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