

Glutaric acid, 8-chlorooctyl 2-hexyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C19H35ClO4/c1-3-4-12-17(2)24-19(22)14-11-13-18(21)23-16-10-8-6-5-7-9-15 |
| InchiKey: | MATDQASIYIJHJQ-UHFFFAOYSA-N |
| Formula: | C19H35ClO4 |
| SMILES: | CCCCC(C)OC(=O)CCCC(=O)OCCCCCCCCCl |
| Mol. weight [g/mol]: | 362.93 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -373.11 | kJ/mol | Joback Method |
| hf | -946.11 | kJ/mol | Joback Method |
| hfus | 51.21 | kJ/mol | Joback Method |
| hvap | 80.20 | kJ/mol | Joback Method |
| log10ws | -5.77 | | Crippen Method |
| logp | 5.401 | | Crippen Method |
| mvol | 305.690 | ml/mol | McGowan Method |
| pc | 1126.83 | kPa | Joback Method |
| rinpol | 2467.00 | | NIST Webbook |
| rinpol | 2467.00 | | NIST Webbook |
| tb | 823.69 | K | Joback Method |
| tc | 1011.93 | K | Joback Method |
| tf | 463.13 | K | Joback Method |
| vc | 1.190 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 941.05 | J/mol×K | 823.69 | Joback Method |
| cpg | 958.06 | J/mol×K | 855.06 | Joback Method |
| cpg | 974.02 | J/mol×K | 886.44 | Joback Method |
| cpg | 988.97 | J/mol×K | 917.81 | Joback Method |
| cpg | 1002.91 | J/mol×K | 949.19 | Joback Method |
| cpg | 1015.87 | J/mol×K | 980.56 | Joback Method |
| cpg | 1027.85 | J/mol×K | 1011.93 | Joback Method |
| dvisc | 0.0008626 | Paxs | 463.13 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0004054 | Paxs | 523.22 | Joback Method |
| dvisc | 0.0002226 | Paxs | 583.32 | Joback Method |
| dvisc | 0.0001367 | Paxs | 643.41 | Joback Method |
| dvisc | 0.0000912 | Paxs | 703.50 | Joback Method |
| dvisc | 0.0000649 | Paxs | 763.60 | Joback Method |
| dvisc | 0.0000485 | Paxs | 823.69 | 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=U393606&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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