

Glutaric acid, decyl 2,5-dimethylphenyl ester

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| Inchi: | InChI=1S/C23H36O4/c1-4-5-6-7-8-9-10-11-17-26-22(24)13-12-14-23(25)27-21-18-19(2) |
| InchiKey: | RKXRAWXSQSMIIOU-UHFFFAOYSA-N |
| Formula: | C23H36O4 |
| SMILES: | CCCCCCCCCOC(=O)CCCC(=O)Oc1cc(C)ccc1C |
| Mol. weight [g/mol]: | 376.53 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -231.91 | kJ/mol | Joback Method |
| hf | -794.06 | kJ/mol | Joback Method |
| hfus | 54.16 | kJ/mol | Joback Method |
| hvap | 88.70 | kJ/mol | Joback Method |
| log10ws | -7.04 | | Crippen Method |
| logp | 6.063 | | Crippen Method |
| mcvol | 326.050 | ml/mol | McGowan Method |
| pc | 1087.06 | kPa | Joback Method |
| rinqol | 2789.00 | | NIST Webbook |
| tb | 914.86 | K | Joback Method |
| tc | 1121.86 | K | Joback Method |
| tf | 544.75 | K | Joback Method |
| vc | 1.264 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1057.52 | J/molxK | 914.86 | Joback Method |
| cpg | 1074.21 | J/molxK | 949.36 | Joback Method |
| cpg | 1089.60 | J/molxK | 983.86 | Joback Method |
| cpg | 1103.70 | J/molxK | 1018.36 | Joback Method |
| cpg | 1116.54 | J/molxK | 1052.86 | Joback Method |
| cpg | 1128.16 | J/molxK | 1087.36 | Joback Method |
| cpg | 1138.58 | J/molxK | 1121.86 | Joback Method |
| dvisc | 0.0003755 | Paxs | 544.75 | Joback Method |
| dvisc | 0.0002088 | Paxs | 606.43 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001294 | Paxs | 668.12 | Joback Method |
| dvisc | 0.0000869 | Paxs | 729.80 | Joback Method |
| dvisc | 0.0000621 | Paxs | 791.49 | Joback Method |
| dvisc | 0.0000466 | Paxs | 853.17 | Joback Method |
| dvisc | 0.0000364 | Paxs | 914.86 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U358943&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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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