

Glutaric acid, decyl 3-phenoxybenzyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C28H38O5/c1-2-3-4-5-6-7-8-12-21-31-27(29)19-14-20-28(30)32-23-24-15-13- |
| InchiKey: | CBUQBNNFFGUWANU-UHFFFAOYSA-N |
| Formula: | C28H38O5 |
| SMILES: | CCCCCCCCCOC(=O)CCCC(=O)OCc1cccc(Oc2ccccc2)c1 |
| Mol. weight [g/mol]: | 454.60 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -172.77 | kJ/mol | Joback Method |
| hf | -781.48 | kJ/mol | Joback Method |
| hfus | 62.73 | kJ/mol | Joback Method |
| hvap | 103.86 | kJ/mol | Joback Method |
| log10ws | -7.99 | | Crippen Method |
| logp | 7.376 | | Crippen Method |
| mcvol | 378.610 | ml/mol | McGowan Method |
| pc | 986.40 | kPa | Joback Method |
| rinpol | 3495.00 | | NIST Webbook |
| tb | 1073.38 | K | Joback Method |
| tc | 1314.79 | K | Joback Method |
| tf | 637.23 | K | Joback Method |
| vc | 1.454 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1286.96 | J/molxK | 1073.38 | Joback Method |
| cpg | 1300.49 | J/molxK | 1113.61 | Joback Method |
| cpg | 1312.16 | J/molxK | 1153.85 | Joback Method |
| cpg | 1322.05 | J/molxK | 1194.08 | Joback Method |
| cpg | 1330.22 | J/molxK | 1234.32 | Joback Method |
| cpg | 1336.74 | J/molxK | 1274.55 | Joback Method |
| cpg | 1341.67 | J/molxK | 1314.79 | Joback Method |
| dvisc | 0.0001460 | Paxs | 637.23 | Joback Method |
| dvisc | 0.0000790 | Paxs | 709.92 | Joback Method |

| | | | | |
|-------|-----------|------|---------|---------------|
| dvisc | 0.0000479 | Paxs | 782.61 | Joback Method |
| dvisc | 0.0000316 | Paxs | 855.30 | Joback Method |
| dvisc | 0.0000223 | Paxs | 928.00 | Joback Method |
| dvisc | 0.0000165 | Paxs | 1000.69 | Joback Method |
| dvisc | 0.0000128 | Paxs | 1073.38 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U358519&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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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