

Glutaric acid, dodecyl 3-methoxybenzyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C25H40O5/c1-3-4-5-6-7-8-9-10-11-12-19-29-24(26)17-14-18-25(27)30-21-22-

OJRNUDXRKTVKQD-UHFFFAOYSA-N

C25H40O5

CCCCCCCCCCCCOC(=O)CCCC(=O)OCc1cccc(OC)c1

420.58

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -310.44 | kJ/mol | Joback Method |
| hf | -956.09 | kJ/mol | Joback Method |
| hfus | 60.92 | kJ/mol | Joback Method |
| hvap | 94.90 | kJ/mol | Joback Method |
| log10ws | -7.31 | | Crippen Method |
| logp | 6.373 | | Crippen Method |
| mcvol | 360.100 | ml/mol | McGowan Method |
| pc | 960.29 | kPa | Joback Method |
| rinpol | 3150.00 | | NIST Webbook |
| tb | 978.06 | K | Joback Method |
| tc | 1197.84 | K | Joback Method |
| tf | 577.00 | K | Joback Method |
| vc | 1.393 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1210.94 | J/molxK | 978.06 | Joback Method |
| cpg | 1227.53 | J/molxK | 1014.69 | Joback Method |
| cpg | 1242.47 | J/molxK | 1051.32 | Joback Method |
| cpg | 1255.79 | J/molxK | 1087.95 | Joback Method |
| cpg | 1267.54 | J/molxK | 1124.58 | Joback Method |
| cpg | 1277.74 | J/molxK | 1161.21 | Joback Method |
| cpg | 1286.41 | J/molxK | 1197.84 | Joback Method |
| dvisc | 0.0002363 | Paxs | 577.00 | Joback Method |
| dvisc | 0.0001258 | Paxs | 643.84 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000754 | Paxs | 710.69 | Joback Method |
| dvisc | 0.0000493 | Paxs | 777.53 | Joback Method |
| dvisc | 0.0000345 | Paxs | 844.37 | Joback Method |
| dvisc | 0.0000255 | Paxs | 911.22 | Joback Method |
| dvisc | 0.0000196 | Paxs | 978.06 | 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=U377197&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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