

Glutaric acid, dodecyl 3-iodobenzyl ester

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|-----------------------------|-----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C24H37IO4/c1-2-3-4-5-6-7-8-9-10-11-18-28-23(26)16-13-17-24(27)29-20-21-1 |
| InchiKey: | YNSMIRGJGTZUOF-UHFFFAOYSA-N |
| Formula: | C24H37IO4 |
| SMILES: | CCCCCCCCCCCCOC(=O)CCCC(=O)OCc1cccc(I)c1 |
| Mol. weight [g/mol]: | 516.45 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -155.74 | kJ/mol | Joback Method |
| hf | -726.36 | kJ/mol | Joback Method |
| hfus | 61.55 | kJ/mol | Joback Method |
| hvap | 99.64 | kJ/mol | Joback Method |
| log10ws | -8.34 | | Crippen Method |
| logp | 6.969 | | Crippen Method |
| mvol | 365.960 | ml/mol | McGowan Method |
| pc | 1016.83 | kPa | Joback Method |
| rinpol | 3337.00 | | NIST Webbook |
| rinpol | 3337.00 | | NIST Webbook |
| tb | 1025.90 | K | Joback Method |
| tc | 1256.07 | K | Joback Method |
| tf | 601.56 | K | Joback Method |
| vc | 1.407 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1170.90 | J/molxK | 1025.90 | Joback Method |
| cpg | 1185.60 | J/molxK | 1064.26 | Joback Method |
| cpg | 1198.92 | J/molxK | 1102.62 | Joback Method |
| cpg | 1210.92 | J/molxK | 1140.98 | Joback Method |
| cpg | 1221.67 | J/molxK | 1179.34 | Joback Method |
| cpg | 1231.22 | J/molxK | 1217.71 | Joback Method |
| cpg | 1239.64 | J/molxK | 1256.07 | Joback Method |
| dvisc | 0.0002534 | Paxs | 601.56 | Joback Method |

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|-------|-----------|------|---------|---------------|
| dvisc | 0.0001340 | Paxs | 672.28 | Joback Method |
| dvisc | 0.0000800 | Paxs | 743.01 | Joback Method |
| dvisc | 0.0000522 | Paxs | 813.73 | Joback Method |
| dvisc | 0.0000365 | Paxs | 884.45 | Joback Method |
| dvisc | 0.0000269 | Paxs | 955.18 | Joback Method |
| dvisc | 0.0000207 | Paxs | 1025.90 | 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=U376992&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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<https://www.chemeo.com/cid/95-568-7/Glutaric-acid-dodecyl-3-iodobenzyl-ester.pdf>

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