

Glutaric acid, oct-1-en-3-yl dec-2-yl ester

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| Inchi: | InChI=1S/C23H42O4/c1-5-8-10-11-12-14-16-20(4)26-22(24)18-15-19-23(25)27-21(7-3)1 |
| InchiKey: | ACUSFSOJZSCPNC-UHFFFAOYSA-N |
| Formula: | C23H42O4 |
| SMILES: | C=CC(CCCCC)OC(=O)CCCC(=O)OC(C)CCCCCCCC |
| Mol. weight [g/mol]: | 382.58 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -242.10 | kJ/mol | Joback Method |
| hf | -892.78 | kJ/mol | Joback Method |
| hfus | 52.57 | kJ/mol | Joback Method |
| hvap | 83.66 | kJ/mol | Joback Method |
| log10ws | -7.25 | | Crippen Method |
| logp | 6.517 | | Crippen Method |
| mvol | 345.510 | ml/mol | McGowan Method |
| pc | 931.78 | kPa | Joback Method |
| rinpol | 2398.00 | | NIST Webbook |
| rinpol | 2398.00 | | NIST Webbook |
| tb | 874.02 | K | Joback Method |
| tc | 1070.15 | K | Joback Method |
| tf | 461.53 | K | Joback Method |
| vc | 1.341 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1126.98 | J/molxK | 874.02 | Joback Method |
| cpg | 1146.01 | J/molxK | 906.71 | Joback Method |
| cpg | 1163.78 | J/molxK | 939.40 | Joback Method |
| cpg | 1180.33 | J/molxK | 972.09 | Joback Method |
| cpg | 1195.70 | J/molxK | 1004.77 | Joback Method |
| cpg | 1209.90 | J/molxK | 1037.46 | Joback Method |
| cpg | 1222.98 | J/molxK | 1070.15 | Joback Method |
| dvisc | 0.0008306 | Paxs | 461.53 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0003359 | Paxs | 530.28 | Joback Method |
| dvisc | 0.0001672 | Paxs | 599.03 | Joback Method |
| dvisc | 0.0000961 | Paxs | 667.77 | Joback Method |
| dvisc | 0.0000612 | Paxs | 736.52 | Joback Method |
| dvisc | 0.0000421 | Paxs | 805.27 | Joback Method |
| dvisc | 0.0000308 | Paxs | 874.02 | 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=U405355&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 |

Latest version available from:

<https://www.chemeo.com/cid/81-646-5/Glutaric-acid-oct-1-en-3-yl-dec-2-yl-ester.pdf>

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