

Glutaric acid, but-3-en-2-yl ethyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C11H18O4/c1-4-9(3)15-11(13)8-6-7-10(12)14-5-2/h4,9H,1,5-8H2,2-3H3 |
| InchiKey: | FHPJEMVMESROQH-UHFFFAOYSA-N |
| Formula: | C11H18O4 |
| SMILES: | <chem>C=CC(C)OC(=O)CCCC(=O)OCC</chem> |
| Mol. weight [g/mol]: | 214.26 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -340.70 | kJ/mol | Joback Method |
| hf | -639.82 | kJ/mol | Joback Method |
| hfus | 25.02 | kJ/mol | Joback Method |
| hvap | 57.33 | kJ/mol | Joback Method |
| log10ws | -2.12 | | Crippen Method |
| logp | 1.837 | | Crippen Method |
| mcvol | 176.430 | ml/mol | McGowan Method |
| pc | 2200.01 | kPa | Joback Method |
| rinpola | 1360.00 | | NIST Webbook |
| tb | 599.90 | K | Joback Method |
| tc | 784.60 | K | Joback Method |
| tf | 341.29 | K | Joback Method |
| vc | 0.674 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 444.35 | J/molxK | 599.90 | Joback Method |
| cpg | 457.97 | J/molxK | 630.68 | Joback Method |
| cpg | 470.98 | J/molxK | 661.47 | Joback Method |
| cpg | 483.37 | J/molxK | 692.25 | Joback Method |
| cpg | 495.15 | J/molxK | 723.03 | Joback Method |
| cpg | 506.32 | J/molxK | 753.82 | Joback Method |
| cpg | 516.88 | J/molxK | 784.60 | Joback Method |
| dvisc | 0.0022154 | Paxs | 341.29 | Joback Method |
| dvisc | 0.0011277 | Paxs | 384.39 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0006577 | Paxs | 427.49 | Joback Method |
| dvisc | 0.0004234 | Paxs | 470.60 | Joback Method |
| dvisc | 0.0002935 | Paxs | 513.70 | Joback Method |
| dvisc | 0.0002153 | Paxs | 556.80 | Joback Method |
| dvisc | 0.0001652 | Paxs | 599.90 | 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=U405251&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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