

Succinic acid, 2-methylpent-3-yl non-3-en-1-yl ester

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|----------------------|--|
| Inchi: | InChI=1S/C19H34O4/c1-5-7-8-9-10-11-12-15-22-18(20)13-14-19(21)23-17(6-2)16(3)4/h |
| InchiKey: | HJLZFFAPNPNGI-ZHACJKMWSA-N |
| Formula: | C19H34O4 |
| SMILES: | CCCCC=CCCOC(=O)CCC(=O)OC(CC)C(C)C |
| Mol. weight [g/mol]: | 326.47 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -283.40 | kJ/mol | Joback Method |
| hf | -818.43 | kJ/mol | Joback Method |
| hfus | 43.70 | kJ/mol | Joback Method |
| hvap | 75.38 | kJ/mol | Joback Method |
| log10ws | -5.22 | | Crippen Method |
| logp | 4.814 | | Crippen Method |
| mvol | 289.150 | ml/mol | McGowan Method |
| pc | 1203.96 | kPa | Joback Method |
| rinpol | 2117.00 | | NIST Webbook |
| rinpol | 2117.00 | | NIST Webbook |
| tb | 789.98 | K | Joback Method |
| tc | 976.37 | K | Joback Method |
| tf | 413.13 | K | Joback Method |
| vc | 1.115 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 885.08 | J/molxK | 789.98 | Joback Method |
| cpg | 902.61 | J/molxK | 821.05 | Joback Method |
| cpg | 919.15 | J/molxK | 852.11 | Joback Method |
| cpg | 934.72 | J/molxK | 883.18 | Joback Method |
| cpg | 949.36 | J/molxK | 914.24 | Joback Method |
| cpg | 963.08 | J/molxK | 945.31 | Joback Method |
| cpg | 975.91 | J/molxK | 976.37 | Joback Method |
| dvisc | 0.0012655 | Paxs | 413.13 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0005031 | Paxs | 475.94 | Joback Method |
| dvisc | 0.0002480 | Paxs | 538.75 | Joback Method |
| dvisc | 0.0001417 | Paxs | 601.56 | Joback Method |
| dvisc | 0.0000900 | Paxs | 664.36 | Joback Method |
| dvisc | 0.0000618 | Paxs | 727.17 | Joback Method |
| dvisc | 0.0000451 | Paxs | 789.98 | 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=U391093&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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