

Succinic acid, 4-methylbenzyl propyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C15H20O4/c1-3-10-18-14(16)8-9-15(17)19-11-13-6-4-12(2)5-7-13/h4-7H,3,8-1 |
| InchiKey: | RVAUKQCMELZPJE-UHFFFAOYSA-N |
| Formula: | C15H20O4 |
| SMILES: | CCCOC(=O)CCC(=O)OCc1ccc(C)cc1 |
| Mol. weight [g/mol]: | 264.32 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -289.64 | kJ/mol | Joback Method |
| hf | -617.47 | kJ/mol | Joback Method |
| hfus | 33.83 | kJ/mol | Joback Method |
| hvap | 70.23 | kJ/mol | Joback Method |
| log10ws | -3.48 | | Crippen Method |
| logp | 2.772 | | Crippen Method |
| mvol | 213.330 | ml/mol | McGowan Method |
| pc | 1975.31 | kPa | Joback Method |
| rinpol | 1955.00 | | NIST Webbook |
| rinpol | 1955.00 | | NIST Webbook |
| tb | 726.84 | K | Joback Method |
| tc | 930.46 | K | Joback Method |
| tf | 442.07 | K | Joback Method |
| vc | 0.816 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 593.63 | J/molxK | 726.84 | Joback Method |
| cpg | 608.41 | J/molxK | 760.78 | Joback Method |
| cpg | 622.26 | J/molxK | 794.71 | Joback Method |
| cpg | 635.18 | J/molxK | 828.65 | Joback Method |
| cpg | 647.19 | J/molxK | 862.59 | Joback Method |
| cpg | 658.30 | J/molxK | 896.52 | Joback Method |
| cpg | 668.51 | J/molxK | 930.46 | Joback Method |
| dvisc | 0.0009203 | Paxs | 442.07 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0005387 | Paxs | 489.53 | Joback Method |
| dvisc | 0.0003467 | Paxs | 536.99 | Joback Method |
| dvisc | 0.0002396 | Paxs | 584.46 | Joback Method |
| dvisc | 0.0001751 | Paxs | 631.92 | Joback Method |
| dvisc | 0.0001337 | Paxs | 679.38 | Joback Method |
| dvisc | 0.0001057 | Paxs | 726.84 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U381051&Units=SI |
| 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 |

Legend

| | |
|----------------------------|---|
| cp_g: | 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 |
| h_{vap}: | Enthalpy of vaporization at standard conditions |
| log₁₀ws: | Log ₁₀ of Water solubility in mol/l |
| log_p: | 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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