

Succinic acid, di(3-methoxybenzyl) ester

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|-----------------------------|----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C20H22O6/c1-23-17-7-3-5-15(11-17)13-25-19(21)9-10-20(22)26-14-16-6-4-8- |
| InchiKey: | YLRVVCIQQJIXJS-UHFFFAOYSA-N |
| Formula: | C20H22O6 |
| SMILES: | COc1cccc(COC(=O)CCC(=O)OCc2cccc(OC)c2)c1 |
| Mol. weight [g/mol]: | 358.39 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -354.76 | kJ/mol | Joback Method |
| hf | -760.05 | kJ/mol | Joback Method |
| hfus | 42.81 | kJ/mol | Joback Method |
| hvap | 89.12 | kJ/mol | Joback Method |
| log10ws | -4.52 | | Crippen Method |
| logp | 3.271 | | Crippen Method |
| mvol | 271.760 | ml/mol | McGowan Method |
| pc | 1668.70 | kPa | Joback Method |
| rinpol | 2851.00 | | NIST Webbook |
| rinpol | 2851.00 | | NIST Webbook |
| tb | 917.74 | K | Joback Method |
| tc | 1141.32 | K | Joback Method |
| tf | 581.82 | K | Joback Method |
| vc | 1.024 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 834.35 | J/molxK | 917.74 | Joback Method |
| cpg | 882.11 | J/molxK | 1104.06 | Joback Method |
| cpg | 875.56 | J/molxK | 1066.79 | Joback Method |
| cpg | 867.50 | J/molxK | 1029.53 | Joback Method |
| cpg | 857.95 | J/molxK | 992.27 | Joback Method |
| cpg | 846.90 | J/molxK | 955.00 | Joback Method |
| cpg | 887.16 | J/molxK | 1141.32 | Joback Method |
| dvisc | 0.0000321 | Paxs | 917.74 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000401 | Paxs | 861.75 | Joback Method |
| dvisc | 0.0000516 | Paxs | 805.77 | Joback Method |
| dvisc | 0.0000691 | Paxs | 749.78 | Joback Method |
| dvisc | 0.0000968 | Paxs | 693.79 | Joback Method |
| dvisc | 0.0001441 | Paxs | 637.81 | Joback Method |
| dvisc | 0.0002313 | Paxs | 581.82 | 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=U381266&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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