

Succinic acid, 4-chloro-3-methylphenyl 2-naphthylmethyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C22H19ClO4/c1-15-12-19(8-9-20(15)23)27-22(25)11-10-21(24)26-14-16-6-7-1 |
| InchiKey: | IZHNINFIEFKAOU-UHFFFAOYSA-N |
| Formula: | C22H19ClO4 |
| SMILES: | <chem>Cc1cc(OC(=O)CCC(=O)OCc2ccc3ccccc3c2)ccc1Cl</chem> |
| Mol. weight [g/mol]: | 382.84 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -42.83 | kJ/mol | Joback Method |
| hf | -373.03 | kJ/mol | Joback Method |
| hfus | 46.44 | kJ/mol | Joback Method |
| hvap | 95.44 | kJ/mol | Joback Method |
| log10ws | -6.98 | | Crippen Method |
| logp | 5.231 | | Crippen Method |
| mcvol | 280.980 | ml/mol | McGowan Method |
| pc | 1717.45 | kPa | Joback Method |
| rinpol | 3270.00 | | NIST Webbook |
| rinpol | 3270.00 | | NIST Webbook |
| tb | 980.05 | K | Joback Method |
| tc | 1222.80 | K | Joback Method |
| tf | 635.04 | K | Joback Method |
| vc | 1.071 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 834.91 | J/molxK | 980.05 | Joback Method |
| cpg | 846.32 | J/molxK | 1020.51 | Joback Method |
| cpg | 856.58 | J/molxK | 1060.97 | Joback Method |
| cpg | 865.76 | J/molxK | 1101.43 | Joback Method |
| cpg | 873.93 | J/molxK | 1141.88 | Joback Method |
| cpg | 881.18 | J/molxK | 1182.34 | Joback Method |
| cpg | 887.58 | J/molxK | 1222.80 | Joback Method |
| dvisc | 0.0003979 | Paxs | 635.04 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0002721 | Paxs | 692.54 | Joback Method |
| dvisc | 0.0001973 | Paxs | 750.04 | Joback Method |
| dvisc | 0.0001497 | Paxs | 807.54 | Joback Method |
| dvisc | 0.0001179 | Paxs | 865.05 | Joback Method |
| dvisc | 0.0000956 | Paxs | 922.55 | Joback Method |
| dvisc | 0.0000795 | Paxs | 980.05 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U390008&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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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