

Succinic acid, 2,4-dichlorobenzyl propyl ester

| | |
|-----------------------------|---|
| Inchi: | InChI=1S/C14H16Cl2O4/c1-2-7-19-13(17)5-6-14(18)20-9-10-3-4-11(15)8-12(10)16/h3-4, |
| InchiKey: | FMGCXYLNQNTJL-UHFFFAOYSA-N |
| Formula: | C14H16Cl2O4 |
| SMILES: | CCCOC(=O)CCC(=O)OCc1ccc(Cl)cc1Cl |
| Mol. weight [g/mol]: | 319.18 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -331.55 | kJ/mol | Joback Method |
| hf | -639.78 | kJ/mol | Joback Method |
| hfus | 39.25 | kJ/mol | Joback Method |
| hvap | 77.44 | kJ/mol | Joback Method |
| log10ws | -4.38 | | Crippen Method |
| logp | 3.770 | | Crippen Method |
| mcvol | 223.720 | ml/mol | McGowan Method |
| pc | 1987.66 | kPa | Joback Method |
| rinpol | 2184.00 | | NIST Webbook |
| rinpol | 2184.00 | | NIST Webbook |
| tb | 783.80 | K | Joback Method |
| tc | 997.33 | K | Joback Method |
| tf | 503.16 | K | Joback Method |
| vc | 0.858 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 588.93 | J/molxK | 783.80 | Joback Method |
| cpg | 640.45 | J/molxK | 961.74 | Joback Method |
| cpg | 631.97 | J/molxK | 926.15 | Joback Method |
| cpg | 622.58 | J/molxK | 890.56 | Joback Method |
| cpg | 612.28 | J/molxK | 854.98 | Joback Method |
| cpg | 601.07 | J/molxK | 819.39 | Joback Method |
| cpg | 648.04 | J/molxK | 997.33 | Joback Method |
| dvisc | 0.0000958 | Paxs | 783.80 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001186 | Paxs | 737.03 | Joback Method |
| dvisc | 0.0001511 | Paxs | 690.25 | Joback Method |
| dvisc | 0.0001996 | Paxs | 643.48 | Joback Method |
| dvisc | 0.0002752 | Paxs | 596.71 | Joback Method |
| dvisc | 0.0004009 | Paxs | 549.93 | Joback Method |
| dvisc | 0.0006262 | Paxs | 503.16 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U381137&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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 |
| hvap: | Enthalpy of vaporization at standard conditions |
| log₁₀ws: | Log ₁₀ of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| m_{cvol}: | 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 |

Latest version available from:

<https://www.chemeo.com/cid/119-121-5/Succinic-acid-2-4-dichlorobenzyl-propyl-ester.pdf>

Generated by Cheméo on 2024-05-06 23:52:53.767885935 +0000 UTC m=+17328822.688463250.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.