

Succinic acid, 4-biphenyl ethyl ester

Inchi: InChI=1S/C18H18O4/c1-2-21-17(19)12-13-18(20)22-16-10-8-15(9-11-16)14-6-4-3-5-7-14
InchiKey: NNFIVIKVPQPNJO-UHFFFAOYSA-N
Formula: C18H18O4
SMILES: CCOC(=O)CCC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 298.33

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -151.97 | kJ/mol | Joback Method |
| hf | -442.86 | kJ/mol | Joback Method |
| hfus | 35.64 | kJ/mol | Joback Method |
| hvap | 79.19 | kJ/mol | Joback Method |
| log10ws | -4.93 | | Crippen Method |
| logp | 3.602 | | Crippen Method |
| mvol | 231.840 | ml/mol | McGowan Method |
| pc | 2053.03 | kPa | Joback Method |
| rinpol | 2459.00 | | NIST Webbook |
| rinpol | 2459.00 | | NIST Webbook |
| tb | 822.16 | K | Joback Method |
| tc | 1050.77 | K | Joback Method |
| tf | 502.30 | K | Joback Method |
| vc | 0.875 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 668.19 | J/molxK | 822.16 | Joback Method |
| cpg | 682.15 | J/molxK | 860.26 | Joback Method |
| cpg | 694.86 | J/molxK | 898.36 | Joback Method |
| cpg | 706.35 | J/molxK | 936.47 | Joback Method |
| cpg | 716.67 | J/molxK | 974.57 | Joback Method |
| cpg | 725.84 | J/molxK | 1012.67 | Joback Method |
| cpg | 733.89 | J/molxK | 1050.77 | Joback Method |
| dvisc | 0.0006210 | Paxs | 502.30 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003667 | Paxs | 555.61 | Joback Method |
| dvisc | 0.0002375 | Paxs | 608.92 | Joback Method |
| dvisc | 0.0001649 | Paxs | 662.23 | Joback Method |
| dvisc | 0.0001210 | Paxs | 715.54 | Joback Method |
| dvisc | 0.0000926 | Paxs | 768.85 | Joback Method |
| dvisc | 0.0000734 | Paxs | 822.16 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U349687&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 |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

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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