

Succinic acid, 2-chlorophenyl 2-methylbutyl ester

| | |
|----------------------|---|
| Inchi: | InChI=1S/C15H19ClO4/c1-3-11(2)10-19-14(17)8-9-15(18)20-13-7-5-4-6-12(13)16/h4-7,1 |
| InchiKey: | IGERFGJLNKMXQA-UHFFFAOYSA-N |
| Formula: | C15H19ClO4 |
| SMILES: | CCC(C)COC(=O)CCC(=O)Oc1ccccc1Cl |
| Mol. weight [g/mol]: | 298.76 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -304.01 | kJ/mol | Joback Method |
| hf | -638.49 | kJ/mol | Joback Method |
| hfus | 34.51 | kJ/mol | Joback Method |
| hvap | 74.23 | kJ/mol | Joback Method |
| log10ws | -4.02 | | Crippen Method |
| logp | 3.615 | | Crippen Method |
| mcvol | 225.570 | ml/mol | McGowan Method |
| pc | 1925.36 | kPa | Joback Method |
| rinsol | 2124.00 | | NIST Webbook |
| tb | 763.83 | K | Joback Method |
| tc | 974.13 | K | Joback Method |
| tf | 456.99 | K | Joback Method |
| vc | 0.859 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 620.63 | J/molxK | 763.83 | Joback Method |
| cpg | 634.52 | J/molxK | 798.88 | Joback Method |
| cpg | 647.43 | J/molxK | 833.93 | Joback Method |
| cpg | 659.36 | J/molxK | 868.98 | Joback Method |
| cpg | 670.31 | J/molxK | 904.03 | Joback Method |
| cpg | 680.32 | J/molxK | 939.08 | Joback Method |
| cpg | 689.38 | J/molxK | 974.13 | Joback Method |
| dvisc | 0.0008947 | Paxs | 456.99 | Joback Method |
| dvisc | 0.0004991 | Paxs | 508.13 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003097 | Paxs | 559.27 | Joback Method |
| dvisc | 0.0002082 | Paxs | 610.41 | Joback Method |
| dvisc | 0.0001489 | Paxs | 661.55 | Joback Method |
| dvisc | 0.0001117 | Paxs | 712.69 | Joback Method |
| dvisc | 0.0000870 | Paxs | 763.83 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U357548&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 |

Latest version available from:

<https://www.chemeo.com/cid/26-229-9/Succinic-acid-2-chlorophenyl-2-methylbutyl-ester.pdf>

Generated by Cheméo on 2024-04-20 11:13:29.209796056 +0000 UTC m=+15900858.130373368.

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