

Isophthalic acid, hexyl 3-methylbut-2-en-1-yl ester

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|----------------------|---|
| Inchi: | InChI=1S/C19H26O4/c1-4-5-6-7-12-22-18(20)16-9-8-10-17(14-16)19(21)23-13-11-15(2)3 |
| InchiKey: | YNNIZWILVAJUEW-UHFFFAOYSA-N |
| Formula: | C19H26O4 |
| SMILES: | CCCCCOC(=O)c1cccc(C(=O)OCC=C(C)C)c1 |
| Mol. weight [g/mol]: | 318.41 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -184.29 | kJ/mol | Joback Method |
| hf | -592.60 | kJ/mol | Joback Method |
| hfus | 43.08 | kJ/mol | Joback Method |
| hvap | 79.18 | kJ/mol | Joback Method |
| log10ws | -5.58 | | Crippen Method |
| logp | 4.547 | | Crippen Method |
| mvol | 265.390 | ml/mol | McGowan Method |
| pc | 1505.81 | kPa | Joback Method |
| rinpol | 2448.00 | | NIST Webbook |
| rinpol | 2448.00 | | NIST Webbook |
| tb | 822.40 | K | Joback Method |
| tc | 1028.52 | K | Joback Method |
| tf | 468.11 | K | Joback Method |
| vc | 1.020 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 792.70 | J/mol×K | 822.40 | Joback Method |
| cpg | 808.27 | J/mol×K | 856.75 | Joback Method |
| cpg | 822.78 | J/mol×K | 891.11 | Joback Method |
| cpg | 836.27 | J/mol×K | 925.46 | Joback Method |
| cpg | 848.77 | J/mol×K | 959.82 | Joback Method |
| cpg | 860.31 | J/mol×K | 994.17 | Joback Method |
| cpg | 870.92 | J/mol×K | 1028.52 | 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=U343938&Units=SI |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvpap: | 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 |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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