

Diethylmalonic acid, hexyl 5-methylhex-2-yl ester

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|----------------------|---|
| Inchi: | InChI=1S/C20H38O4/c1-7-10-11-12-15-23-18(21)20(8-2,9-3)19(22)24-17(6)14-13-16(4)5 |
| InchiKey: | DLBWSRIAINFMEH-UHFFFAOYSA-N |
| Formula: | C20H38O4 |
| SMILES: | CCCCCOC(=O)C(CC)(CC)C(=O)OC(C)CCC(C)C |
| Mol. weight [g/mol]: | 342.51 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -352.36 | kJ/mol | Joback Method |
| hf | -965.04 | kJ/mol | Joback Method |
| hfus | 38.67 | kJ/mol | Joback Method |
| hvap | 76.35 | kJ/mol | Joback Method |
| log10ws | -5.55 | | Crippen Method |
| logp | 5.284 | | Crippen Method |
| mcvol | 307.540 | ml/mol | McGowan Method |
| pc | 1103.01 | kPa | Joback Method |
| rinqol | 1982.00 | | NIST Webbook |
| tb | 805.47 | K | Joback Method |
| tc | 993.66 | K | Joback Method |
| tf | 431.90 | K | Joback Method |
| vc | 1.181 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 971.15 | J/molxK | 805.47 | Joback Method |
| cpg | 1052.84 | J/molxK | 962.29 | Joback Method |
| cpg | 1038.57 | J/molxK | 930.93 | Joback Method |
| cpg | 1023.29 | J/molxK | 899.56 | Joback Method |
| cpg | 1006.98 | J/molxK | 868.20 | Joback Method |
| cpg | 989.61 | J/molxK | 836.83 | Joback Method |
| cpg | 1066.15 | J/molxK | 993.66 | Joback Method |
| dvisc | 0.0000360 | Paxs | 805.47 | Joback Method |
| dvisc | 0.0000505 | Paxs | 743.21 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000753 | Paxs | 680.95 | Joback Method |
| dvisc | 0.0001216 | Paxs | 618.68 | Joback Method |
| dvisc | 0.0002188 | Paxs | 556.42 | Joback Method |
| dvisc | 0.0004564 | Paxs | 494.16 | Joback Method |
| dvisc | 0.0011766 | Paxs | 431.90 | 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=U369298&Units=SI |

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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