

Dibenzo[b,tuv]naphtho[2,1-m]picene

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|-----------------------------|---|
| Inchi: | InChI=1S/C36H20/c1-3-7-25-21(5-1)9-12-28-27(25)15-17-30-29(28)16-18-31-33-14-10-2 |
| InchiKey: | DSPSAZHJBQSTMS-UHFFFAOYSA-N |
| Formula: | C36H20 |
| SMILES: | <chem>c1ccc2c(c1)ccc1c2ccc2c1ccc1c2cc2ccc3c4ccccc4cc4ccc1c2c43</chem> |
| Mol. weight [g/mol]: | 452.54 |
| CAS: | 13354-54-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 1144.68 | kJ/mol | Joback Method |
| hf | 852.97 | kJ/mol | Joback Method |
| hfus | 59.44 | kJ/mol | Joback Method |
| hvap | 115.12 | kJ/mol | Joback Method |
| log10ws | -15.32 | | Crippen Method |
| logp | 10.350 | | Crippen Method |
| mcvol | 342.960 | ml/mol | McGowan Method |
| pc | 1509.33 | kPa | Joback Method |
| tb | 1228.76 | K | Joback Method |
| tc | 1519.31 | K | Joback Method |
| tf | 877.42 | K | Joback Method |
| vc | 1.349 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1176.13 | J/molxK | 1228.76 | Joback Method |
| cpg | 1425.02 | J/molxK | 1470.89 | Joback Method |
| cpg | 1362.92 | J/molxK | 1422.46 | Joback Method |
| cpg | 1307.64 | J/molxK | 1374.04 | Joback Method |
| cpg | 1258.52 | J/molxK | 1325.61 | Joback Method |
| cpg | 1214.90 | J/molxK | 1277.19 | Joback Method |
| cpg | 1494.62 | J/molxK | 1519.31 | Joback Method |
| dvisc | 0.0184030 | Paxs | 1228.76 | Joback Method |
| dvisc | 0.0189069 | Paxs | 1170.20 | Joback Method |

| | | | | |
|-------|-----------|------|---------|---------------|
| dvisc | 0.0194799 | Paxs | 1111.65 | Joback Method |
| dvisc | 0.0201371 | Paxs | 1053.09 | Joback Method |
| dvisc | 0.0208980 | Paxs | 994.53 | Joback Method |
| dvisc | 0.0217885 | Paxs | 935.98 | Joback Method |
| dvisc | 0.0228438 | Paxs | 877.42 | 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=C13354546&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 |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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