

Tribenzo[a,hi,kl]coronene

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|-----------------------------|---|
| Inchi: | InChI=1S/C34H16/c1-2-8-22-21(7-1)25-13-11-19-15-17-5-3-9-23-24-10-4-6-18-16-20-12 |
| InchiKey: | IZPWQXVAQIDTTK-UHFFFAOYSA-N |
| Formula: | C34H16 |
| SMILES: | <chem>c1ccc2c(c1)c1ccc3cc4cccc5c6cccc7cc8ccc2c2c8c(c76)c(c45)c3c12</chem> |
| Mol. weight [g/mol]: | 424.49 |
| CAS: | 128345-67-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 1207.58 | kJ/mol | Joback Method |
| hf | 937.47 | kJ/mol | Joback Method |
| hfus | 59.83 | kJ/mol | Joback Method |
| hvap | 111.07 | kJ/mol | Joback Method |
| log10ws | -15.37 | | Crippen Method |
| logp | 9.817 | | Crippen Method |
| mcvol | 308.220 | ml/mol | McGowan Method |
| pc | 1721.73 | kPa | Joback Method |
| tb | 1183.86 | K | Joback Method |
| tc | 1465.19 | K | Joback Method |
| tf | 918.94 | K | Joback Method |
| vc | 1.250 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1044.98 | J/molxK | 1183.86 | Joback Method |
| cpg | 1321.06 | J/molxK | 1418.30 | Joback Method |
| cpg | 1251.03 | J/molxK | 1371.42 | Joback Method |
| cpg | 1189.14 | J/molxK | 1324.53 | Joback Method |
| cpg | 1134.65 | J/molxK | 1277.64 | Joback Method |
| cpg | 1086.84 | J/molxK | 1230.75 | Joback Method |
| cpg | 1399.93 | J/molxK | 1465.19 | Joback Method |
| dvisc | 0.4969759 | Paxs | 1183.86 | Joback Method |
| dvisc | 0.4830780 | Paxs | 1139.71 | Joback Method |

| | | | | |
|-------|-----------|------|---------|---------------|
| dvisc | 0.4684964 | Paxs | 1095.55 | Joback Method |
| dvisc | 0.4531868 | Paxs | 1051.40 | Joback Method |
| dvisc | 0.4371025 | Paxs | 1007.25 | Joback Method |
| dvisc | 0.4201945 | Paxs | 963.09 | Joback Method |
| dvisc | 0.4024121 | Paxs | 918.94 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C128345675&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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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