

Naphth[2',1'!4,5]indeno[1,2,3-cd]pyrene

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|-----------------------------|---|
| Other names: | Naphth[2',1':4,5]indeno[1,2,3-cd]pyrene |
| Inchi: | InChI=1S/C30H16/c1-2-5-20-15-25-21(14-19(20)4-1)11-13-23-24-12-10-18-9-8-17-6-3-7 |
| InchiKey: | LFRIIMQTTMOUKG-UHFFFAOYSA-N |
| Formula: | C30H16 |
| SMILES: | <chem>c1ccc2cc3c4c(ccc3cc2c1)-c1ccc2ccc3cccc5cc-4c1c2c35</chem> |
| Mol. weight [g/mol]: | 376.45 |
| CAS: | 106404-29-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 991.38 | kJ/mol | Joback Method |
| hf | 751.75 | kJ/mol | Joback Method |
| hfus | 50.25 | kJ/mol | Joback Method |
| hvap | 98.83 | kJ/mol | Joback Method |
| log10ws | -13.36 | | Crippen Method |
| logp | 8.538 | | Crippen Method |
| mcvol | 282.180 | ml/mol | McGowan Method |
| pc | 1867.55 | kPa | Joback Method |
| tb | 1059.82 | K | Joback Method |
| tc | 1334.83 | K | Joback Method |
| tf | 770.86 | K | Joback Method |
| vc | 1.121 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 877.53 | J/molxK | 1059.82 | Joback Method |
| cpg | 1022.37 | J/molxK | 1288.99 | Joback Method |
| cpg | 986.42 | J/molxK | 1243.16 | Joback Method |
| cpg | 954.48 | J/molxK | 1197.32 | Joback Method |
| cpg | 926.04 | J/molxK | 1151.49 | Joback Method |
| cpg | 900.56 | J/molxK | 1105.65 | Joback Method |
| cpg | 1062.84 | J/molxK | 1334.83 | Joback Method |
| dvisc | 0.0266349 | Paxs | 1059.82 | Joback Method |

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|-------|-----------|------|---------|---------------|
| dvisc | 0.0267743 | Paxs | 1011.66 | Joback Method |
| dvisc | 0.0269285 | Paxs | 963.50 | Joback Method |
| dvisc | 0.0270999 | Paxs | 915.34 | Joback Method |
| dvisc | 0.0272917 | Paxs | 867.18 | Joback Method |
| dvisc | 0.0275076 | Paxs | 819.02 | Joback Method |
| dvisc | 0.0277526 | Paxs | 770.86 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C106404299&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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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