

1,4:5,8:9,10-Trimethanoanthracene, 1,2,3,4,4a,5,8,8a,9,9a,10,10a-dodecahydro-(1 «alpha

Inchi: InChI=1S/C17H22/c1-2-9-5-8(1)14-12-7-13(15(9)14)17-11-4-3-10(6-11)16(12)17/h1-2,8-
InchiKey: FUCGLOJSPSEIKX-DTSMRLRQCSA-N
Formula: C17H22
SMILES: C1=CC2CC1C1C3CC(C21)C1C2CCC(C2)C31
Mol. weight [g/mol]: 226.36
CAS: 87480-43-1

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 467.98 | kJ/mol | Joback Method |
| hf | 25.17 | kJ/mol | Joback Method |
| hfus | 36.20 | kJ/mol | Joback Method |
| hvap | 51.80 | kJ/mol | Joback Method |
| ie | 8.47 | eV | NIST Webbook |
| log10ws | -3.74 | | Crippen Method |
| logp | 3.737 | | Crippen Method |
| mcvol | 180.930 | ml/mol | McGowan Method |
| pc | 2083.12 | kPa | Joback Method |
| tb | 605.01 | K | Joback Method |
| tc | 828.43 | K | Joback Method |
| tf | 376.31 | K | Joback Method |
| vc | 0.720 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 569.82 | J/molxK | 605.01 | Joback Method |
| cpg | 676.51 | J/molxK | 791.19 | Joback Method |
| cpg | 658.01 | J/molxK | 753.95 | Joback Method |
| cpg | 638.31 | J/molxK | 716.72 | Joback Method |
| cpg | 617.19 | J/molxK | 679.48 | Joback Method |
| cpg | 594.43 | J/molxK | 642.25 | Joback Method |
| cpg | 694.04 | J/molxK | 828.43 | Joback Method |
| dvisc | 0.0627123 | Paxs | 605.01 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0475853 | Paxs | 566.89 | Joback Method |
| dvisc | 0.0346984 | Paxs | 528.78 | Joback Method |
| dvisc | 0.0240900 | Paxs | 490.66 | Joback Method |
| dvisc | 0.0157277 | Paxs | 452.54 | Joback Method |
| dvisc | 0.0094937 | Paxs | 414.43 | Joback Method |
| dvisc | 0.0051736 | Paxs | 376.31 | Joback Method |

Sources

| | |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| 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=C87480431&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|----------------------------|-------------------------------------------------|
| cp_g: | 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 |
| ie: | Ionization energy |
| log₁₀ws: | Log ₁₀ of Water solubility in mol/l |
| log_p: | 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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