Phenanthrene, 9-dodecyl-

Other names: 9-n-Dodecylphenanthrene
9-Dodecylphenathrene
Inchi: InChI=1S/C26H34/c1-2-3-4-5-6-7-8-9-10-11-16-22-21-23-17-12-13-18-24(23)26-20-15-14
InchiKey: QBNLPAPGLLSKBN-UHFFFAOYSA-N
Formula: C26H34
SMILES: CCCCCCCCCCCCc1cc2ccccc2c2ccccc12
Mol. weight [g/mol]: 346.55
CAS: 3788-61-2

Physical Properties

Property code	Value	Unit	Source
gf	474.49	kJ/mol	Joback Method
hf	15.76	kJ/mol	Joback Method
hfus	50.40	kJ/mol	Joback Method
hvap	80.35	kJ/mol	Joback Method
log10ws	-10.07		Crippen Method
logp	8.456		Crippen Method
mcvol	314.520	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
tb	868.88	K	Joback Method
tc	1081.32	K	Joback Method
tf	348.95 ± 0.50	K	NIST Webbook
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1090.04	J/mol×K	1081.32	Joback Method
cpg	1074.90	J/mol×K	1045.91	Joback Method
cpg	1059.27	J/mol×K	1010.51	Joback Method
cpg	1043.04	J/mol×K	975.10	Joback Method
cpg	1026.10	J/mol×K	939.69	Joback Method
cpg	1008.32	J/mol×K	904.29	Joback Method
cpg	989.60	J/mol×K	868.88	Joback Method

dvisc	0.0010828	Pa×s	499.64	Joback Method
dvisc	0.0001824	Pa×s	868.88	Joback Method
dvisc	0.0002191	Pa×s	807.34	Joback Method
dvisc	0.0002715	Pa×s	745.80	Joback Method
dvisc	0.0003494	Pa×s	684.26	Joback Method
dvisc	0.0004729	Pa×s	622.72	Joback Method
dvisc	0.0006838	Pa×s	561.18	Joback Method
hvapt	95.70	kJ/mol	531.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3788612&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
hvapt: Enthalpy of vaporization at a given temperature
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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