

Phenanthrene, 2-dodecyl-

Other names:	2-Dodecylphenanthrene 2-n-Dodecylphenanthrene
Inchi:	InChI=1S/C26H34/c1-2-3-4-5-6-7-8-9-10-11-14-22-17-20-26-24(21-22)19-18-23-15-12-1
InchiKey:	STXCMFGUPUBXHF-UHFFFAOYSA-N
Formula:	C26H34
SMILES:	CCCCCCCCCCCCc1ccc2c(ccc3ccccc32)c1
Mol. weight [g/mol]:	346.55
CAS:	3674-72-4

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
mvol	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	499.64	K	Joback Method
vc	1.228	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001824	Paxs	868.88	Joback Method
dvisc	0.0002191	Paxs	807.34	Joback Method
dvisc	0.0002715	Paxs	745.80	Joback Method
dvisc	0.0003494	Paxs	684.26	Joback Method
dvisc	0.0004729	Paxs	622.72	Joback Method
dvisc	0.0006838	Paxs	561.18	Joback Method
dvisc	0.0010828	Paxs	499.64	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=C3674724&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
hvac:	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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