

Phenanthrene, 9-dodecyltetradecahydro-

Other names:	9-n-Dodecylperhydrophenanthrene 9-n-Dodecyl(tetradecahydrophenanthrene) 9-Dodecyltetrahydrophenanthrene
Inchi:	InChI=1S/C26H48/c1-2-3-4-5-6-7-8-9-10-11-16-22-21-23-17-12-13-18-24(23)26-20-15-1
InchiKey:	JTVJHJFIEIFWQH-UHFFFAOYSA-N
Formula:	C26H48
SMILES:	CCCCCCCCCCCC1CC2CCCCC2C2CCCC12
Mol. weight [g/mol]:	360.66
CAS:	55334-01-5

Physical Properties

Property code	Value	Unit	Source
gf	274.37	kJ/mol	Joback Method
hf	-433.05	kJ/mol	Joback Method
hfus	49.14	kJ/mol	Joback Method
hvap	73.45	kJ/mol	Joback Method
log10ws	-9.18		Crippen Method
logp	8.930		Crippen Method
mcvol	344.620	ml/mol	McGowan Method
pc	938.07	kPa	Joback Method
tb	826.51	K	Joback Method
tc	1026.96	K	Joback Method
tf	410.52	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1203.39	J/mol×K	826.51	Joback Method
cpg	1229.34	J/mol×K	859.92	Joback Method
cpg	1253.73	J/mol×K	893.33	Joback Method
cpg	1276.64	J/mol×K	926.73	Joback Method
cpg	1298.15	J/mol×K	960.14	Joback Method
cpg	1318.36	J/mol×K	993.55	Joback Method

cpg	1337.35	J/mol×K	1026.96	Joback Method
dvisc	0.0030069	Pa×s	410.52	Joback Method
dvisc	0.0016056	Pa×s	479.85	Joback Method
dvisc	0.0010045	Pa×s	549.18	Joback Method
dvisc	0.0006982	Pa×s	618.51	Joback Method
dvisc	0.0005222	Pa×s	687.85	Joback Method
dvisc	0.0004119	Pa×s	757.18	Joback Method
dvisc	0.0003380	Pa×s	826.51	Joback Method
hvapt	90.80	kJ/mol	522.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55334015&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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