Perhydrophenanthrene, 1B-(3R-methylhexyl)-2A,4bB,8,8,10aB-pentamethy

Inchi: InChI=1S/C26H48/c1-8-10-19(2)11-13-21-20(3)12-14-23-25(21,6)18-15-22-24(4,5)16-9-1

InchiKey: LDBHPHKACOKILM-WYZVDPMTSA-N

Formula: C26H48

SMILES: CCCC(C)CCC1C(C)CCC2C1(C)CCC1C(C)(C)CCCC12C

Mol. weight [g/mol]: 360.66

Physical Properties

Property code	Value	Unit	Source
gf	240.04	kJ/mol	Joback Method
hf	-433.29	kJ/mol	Joback Method
hfus	28.87	kJ/mol	Joback Method
hvap	68.99	kJ/mol	Joback Method
log10ws	-8.46		Crippen Method
logp	8.498		Crippen Method
mcvol	344.620	ml/mol	McGowan Method
pc	983.93	kPa	Joback Method
rinpol	2594.00		NIST Webbook
tb	817.45	K	Joback Method
tc	1033.34	K	Joback Method
tf	458.74	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1195.20	J/mol×K	817.45	Joback Method
cpg	1226.86	J/mol×K	853.43	Joback Method
cpg	1258.38	J/mol×K	889.41	Joback Method
cpg	1290.09	J/mol×K	925.39	Joback Method
cpg	1322.35	J/mol×K	961.37	Joback Method
cpg	1355.48	J/mol×K	997.36	Joback Method
cpg	1389.85	J/mol×K	1033.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R556782&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume