Perhydrophenanthrene, 1B-(3S,7-dimethylnonyl)-2A,4bB,8,8,10aB-pentam

Inchi: InChI=1S/C30H56/c1-9-22(2)12-10-13-23(3)14-16-25-24(4)15-17-27-29(25,7)21-18-26-2

InchiKey: LKFHRJUTBBHMDC-WMKZCOPOSA-N

Formula: C30H56

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

Mol. weight [g/mol]: 416.77

Physical Properties

Property code	Value	Unit	Source
gf	271.28	kJ/mol	Joback Method
hf	-521.13	kJ/mol	Joback Method
hfus	35.70	kJ/mol	Joback Method
hvap	77.51	kJ/mol	Joback Method
log10ws	-9.89		Crippen Method
logp	9.914		Crippen Method
mcvol	400.980	ml/mol	McGowan Method
pc	787.27	kPa	Joback Method
rinpol	3009.00		NIST Webbook
tb	908.53	K	Joback Method
tc	1123.97	K	Joback Method
tf	488.82	K	Joback Method
vc	1.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1473.55	J/mol×K	908.53	Joback Method
cpg	1508.97	J/mol×K	944.44	Joback Method
cpg	1544.87	J/mol×K	980.34	Joback Method
cpg	1581.63	J/mol×K	1016.25	Joback Method
cpg	1619.58	J/mol×K	1052.16	Joback Method
cpg	1659.09	J/mol×K	1088.06	Joback Method
cpg	1700.51	J/mol×K	1123.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R556811&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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