Perhydrophenanthrene, 1B-(3R,7-dimethyloctyl)-2A,4bB,8,8,10aB-pentame

Inchi: InChI=1S/C29H54/c1-21(2)11-9-12-22(3)13-15-24-23(4)14-16-26-28(24,7)20-17-25-27(5

InchiKey: ODDWOZCOVPOZCZ-ROZAETHSSA-N

Formula: C29H54

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

Mol. weight [g/mol]: 402.74

Physical Properties

Property code	Value	Unit	Source
gf	262.86	kJ/mol	Joback Method
hf	-500.49	kJ/mol	Joback Method
hfus	33.12	kJ/mol	Joback Method
hvap	75.28	kJ/mol	Joback Method
log10ws	-9.47		Crippen Method
logp	9.524		Crippen Method
mcvol	386.890	ml/mol	McGowan Method
pc	831.46	kPa	Joback Method
rinpol	2852.00		NIST Webbook
tb	885.65	K	Joback Method
tc	1100.89	K	Joback Method
tf	477.55	K	Joback Method
vc	1.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1402.26	J/mol×K	885.65	Joback Method
cpg	1436.58	J/mol×K	921.52	Joback Method
cpg	1471.23	J/mol×K	957.40	Joback Method
cpg	1506.55	J/mol×K	993.27	Joback Method
cpg	1542.89	J/mol×K	1029.14	Joback Method
cpg	1580.60	J/mol×K	1065.02	Joback Method
cpg	1620.03	J/mol×K	1100.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R556777&Units=SI

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