Perhydrophenanthrene, 1A-isopentyl-2A,4bB,8,8,10aB-pentamethyl

Inchi: InChI=1S/C24H44/c1-17(2)9-11-19-18(3)10-12-21-23(19,6)16-13-20-22(4,5)14-8-15-24(2

InchiKey: NMRHSKVRUWBTQL-BXGXVPBKSA-N

Formula: C24H44

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

Mol. weight [g/mol]: 332.61

Physical Properties

Property code	Value	Unit	Source
gf	223.20	kJ/mol	Joback Method
hf	-392.01	kJ/mol	Joback Method
hfus	23.69	kJ/mol	Joback Method
hvap	64.54	kJ/mol	Joback Method
log10ws	-7.62		Crippen Method
logp	7.718		Crippen Method
mcvol	316.440	ml/mol	McGowan Method
pc	1114.08	kPa	Joback Method
rinpol	2427.00		NIST Webbook
rinpol	2427.00		NIST Webbook
tb	771.69	K	Joback Method
tc	992.50	K	Joback Method
tf	436.20	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.23	J/mol×K	771.69	Joback Method
cpg	1094.00	J/mol×K	808.49	Joback Method
cpg	1124.30	J/mol×K	845.29	Joback Method
cpg	1154.51	J/mol×K	882.09	Joback Method
cpg	1184.97	J/mol×K	918.90	Joback Method
cpg	1216.04	J/mol×K	955.70	Joback Method
cpg	1248.10	J/mol×K	992.50	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=R556737&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