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

Inchi: InChI=1S/C23H42/c1-7-8-10-18-17(2)11-12-20-22(18,5)16-13-19-21(3,4)14-9-15-23(19,2

InchiKey: DANSPNRFCNAGDG-OSXVMJTBSA-N

Formula: C23H42

SMILES: CCCCC1C(C)CCC2C1(C)CCC1C(C)(C)CCCC12C

Mol. weight [g/mol]: 318.58

Physical Properties

Property code	Value	Unit	Source
gf	217.22	kJ/mol	Joback Method
hf	-366.09	kJ/mol	Joback Method
hfus	24.62	kJ/mol	Joback Method
hvap	62.70	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	7.472		Crippen Method
mcvol	302.350	ml/mol	McGowan Method
pc	1182.53	kPa	Joback Method
rinpol	2374.00		NIST Webbook
tb	749.25	K	Joback Method
tc	969.54	K	Joback Method
tf	439.93	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.61	J/mol×K	749.25	Joback Method
cpg	1028.56	J/mol×K	785.96	Joback Method
cpg	1057.92	J/mol×K	822.68	Joback Method
cpg	1087.04	J/mol×K	859.39	Joback Method
cpg	1116.26	J/mol×K	896.11	Joback Method
cpg	1145.95	J/mol×K	932.82	Joback Method
cpg	1176.46	J/mol×K	969.54	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=R556717&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