Perhydrophenanthrene, 1,4bB,8,8,10aB-pentamethyl

Inchi: InChI=1S/C19H34/c1-14-8-6-9-16-18(14,4)13-10-15-17(2,3)11-7-12-19(15,16)5/h14-16H
InchiKey: JAQCKRGOHDLTRL-WFZCBACDSA-N
Formula: C19H34
SMILES: CC1CCCC2C1(C)CCC1C(C)(C)CCCC12C
Mol. weight [g/mol]: 262.47

Physical Properties

Property code	Value	Unit	Source
gf	191.25	kJ/mol	Joback Method
hf	-263.19	kJ/mol	Joback Method
hfus	13.19	kJ/mol	Joback Method
hvap	54.11	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	6.055		Crippen Method
mcvol	245.990	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	1915.00		NIST Webbook
tb	662.40	K	Joback Method
tc	898.99	K	Joback Method
tf	399.09	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.38	J/mol×K	662.40	Joback Method
cpg	781.24	J/mol×K	701.83	Joback Method
cpg	808.84	J/mol×K	741.26	Joback Method
cpg	835.64	J/mol×K	780.69	Joback Method
cpg	862.05	J/mol×K	820.12	Joback Method
cpg	888.51	J/mol×K	859.55	Joback Method
cpg	915.45	J/mol×K	898.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R556653&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

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

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