Perhydrophenanthrene, 1B-(3-methylpentyl)-2A,4bB,8,8,10aB-pentamethy

Inchi: InChI=1S/C25H46/c1-8-18(2)10-12-20-19(3)11-13-22-24(20,6)17-14-21-23(4,5)15-9-16-2

InchiKey: YFMRPILVLYAHKS-GPABRMKCSA-N

Formula: C25H46

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

Mol. weight [g/mol]: 346.63

Physical Properties

Property code	Value	Unit	Source
gf	231.62	kJ/mol	Joback Method
hf	-412.65	kJ/mol	Joback Method
hfus	26.28	kJ/mol	Joback Method
hvap	66.77	kJ/mol	Joback Method
log10ws	-8.04		Crippen Method
logp	8.108		Crippen Method
mcvol	330.530	ml/mol	McGowan Method
pc	1045.97	kPa	Joback Method
rinpol	2508.00		NIST Webbook
tb	794.57	K	Joback Method
tc	1012.63	K	Joback Method
tf	447.47	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1128.63	J/mol×K	794.57	Joback Method
cpg	1159.79	J/mol×K	830.91	Joback Method
cpg	1190.65	J/mol×K	867.26	Joback Method
cpg	1221.55	J/mol×K	903.60	Joback Method
cpg	1252.85	J/mol×K	939.95	Joback Method
cpg	1284.89	J/mol×K	976.29	Joback Method
cpg	1318.04	J/mol×K	1012.63	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=R556742&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