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

Inchi: InChI=1S/C28H52/c1-8-9-10-12-21(2)13-15-23-22(3)14-16-25-27(23,6)20-17-24-26(4,5)1

InchiKey: CLWTVLJDQACLFC-RKHCOYROSA-N

Formula: C28H52

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

Mol. weight [g/mol]: 388.71

Physical Properties

Property code	Value	Unit	Source
gf	256.88	kJ/mol	Joback Method
hf	-474.57	kJ/mol	Joback Method
hfus	34.05	kJ/mol	Joback Method
hvap	73.44	kJ/mol	Joback Method
log10ws	-9.29		Crippen Method
logp	9.278		Crippen Method
mcvol	372.800	ml/mol	McGowan Method
pc	875.32	kPa	Joback Method
rinpol	2806.00		NIST Webbook
tb	863.21	K	Joback Method
tc	1076.62	K	Joback Method
tf	481.28	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1331.86	J/mol×K	863.21	Joback Method
cpg	1364.94	J/mol×K	898.78	Joback Method
cpg	1398.19	J/mol×K	934.35	Joback Method
cpg	1431.95	J/mol×K	969.92	Joback Method
cpg	1466.55	J/mol×K	1005.49	Joback Method
cpg	1502.33	J/mol×K	1041.05	Joback Method
cpg	1539.63	J/mol×K	1076.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R556846&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