Perhydrophenanthrene, 2B,4bB,8,8,10aB-pentamethyl-1A-(3-oxobutyl)

Inchi: InChI=1S/C23H40O/c1-16-8-11-20-22(5,18(16)10-9-17(2)24)15-12-19-21(3,4)13-7-14-23

InchiKey: XNAGUWARFHSTGQ-URTGAJQUSA-N

Formula: C23H40O

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

Mol. weight [g/mol]: 332.56

Physical Properties

Property code	Value	Unit	Source
gf	88.30	kJ/mol	Joback Method
hf	-478.67	kJ/mol	Joback Method
hfus	26.22	kJ/mol	Joback Method
hvap	69.45	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	6.651		Crippen Method
mcvol	303.920	ml/mol	McGowan Method
pc	1235.48	kPa	Joback Method
rinpol	2581.00		NIST Webbook
rinpol	2581.00		NIST Webbook
tb	803.12	K	Joback Method
tc	1029.06	K	Joback Method
tf	489.86	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1034.58	J/mol×K	803.12	Joback Method
cpg	1063.94	J/mol×K	840.78	Joback Method
cpg	1093.22	J/mol×K	878.43	Joback Method
cpg	1122.79	J/mol×K	916.09	Joback Method
cpg	1153.04	J/mol×K	953.75	Joback Method
cpg	1184.34	J/mol×K	991.40	Joback Method
cpg	1217.07	J/mol×K	1029.06	Joback Method

Sources

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=R556935&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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