Perhydrophenanthrene, 2A,4bB,8,8,10aB-pentamethyl-1A-(3R/S-methyl-7-

Inchi: InChI=1S/C28H50O/c1-20(10-8-11-22(3)29)12-14-23-21(2)13-15-25-27(23,6)19-16-24-2

InchiKey: DJTIKPPBMWKDMJ-SGQUFSSSSA-N

Formula: C28H50O

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

Mol. weight [g/mol]: 402.70

Physical Properties

Property code	Value	Unit	Source
gf	127.96	kJ/mol	Joback Method
hf	-587.15	kJ/mol	Joback Method
hfus	35.65	kJ/mol	Joback Method
hvap	80.19	kJ/mol	Joback Method
log10ws	-8.57		Crippen Method
logp	8.457		Crippen Method
mcvol	374.370	ml/mol	McGowan Method
pc	908.89	kPa	Joback Method
rinpol	3075.00		NIST Webbook
rinpol	3075.00		NIST Webbook
tb	917.08	K	Joback Method
tc	1137.68	K	Joback Method
tf	531.21	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1372.45	J/mol×K	917.08	Joback Method
cpg	1406.44	J/mol×K	953.85	Joback Method
cpg	1441.15	J/mol×K	990.61	Joback Method
cpg	1476.94	J/mol×K	1027.38	Joback Method
cpg	1514.20	J/mol×K	1064.15	Joback Method
cpg	1553.28	J/mol×K	1100.92	Joback Method
cpg	1594.57	J/mol×K	1137.68	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=R556915&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