Perhydrophenanthrene, 1A-(3R/S,7-dimethyldecyl)-2A,4bB,8,8,10aB-penta

Inchi: InChI=1S/C31H58/c1-9-12-23(2)13-10-14-24(3)15-17-26-25(4)16-18-28-30(26,7)22-19-2

InchiKey: VUYKMUGBDPHBEV-NMJNTQMDSA-N

Formula: C31H58

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

Mol. weight [g/mol]: 430.79

Physical Properties

Property code	Value	Unit	Source
gf	279.70	kJ/mol	Joback Method
hf	-541.77	kJ/mol	Joback Method
hfus	38.29	kJ/mol	Joback Method
hvap	79.73	kJ/mol	Joback Method
log10ws	-10.31		Crippen Method
logp	10.304		Crippen Method
mcvol	415.070	ml/mol	McGowan Method
pc	746.51	kPa	Joback Method
rinpol	3100.00		NIST Webbook
tb	931.41	K	Joback Method
tc	1147.84	K	Joback Method
tf	500.09	K	Joback Method
vc	1.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1546.08	J/mol×K	931.41	Joback Method
cpg	1582.79	J/mol×K	967.48	Joback Method
cpg	1620.18	J/mol×K	1003.55	Joback Method
cpg	1658.61	J/mol×K	1039.62	Joback Method
cpg	1698.43	J/mol×K	1075.69	Joback Method
cpg	1740.02	J/mol×K	1111.77	Joback Method
cpg	1783.74	J/mol×K	1147.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R556673&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