Perhydrophenanthrene, 1B-ethyl-2B,4bB,8,8,10aB-pentamethyl

Inchi: InChI=1S/C21H38/c1-7-16-15(2)9-10-18-20(16,5)14-11-17-19(3,4)12-8-13-21(17,18)6/h1

InchiKey: WDSHDPRMSZAAGE-NELBKZFDSA-N

Formula: C21H38

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

Mol. weight [g/mol]: 290.53

Physical Properties

Property code	Value	Unit	Source
gf	200.38	kJ/mol	Joback Method
hf	-324.81	kJ/mol	Joback Method
hfus	19.44	kJ/mol	Joback Method
hvap	58.25	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.691		Crippen Method
mcvol	274.170	ml/mol	McGowan Method
pc	1355.63	kPa	Joback Method
rinpol	2112.00		NIST Webbook
rinpol	2112.00		NIST Webbook
tb	703.49	K	Joback Method
tc	931.16	K	Joback Method
tf	417.39	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.62	J/mol×K	703.49	Joback Method
cpg	903.18	J/mol×K	741.43	Joback Method
cpg	931.80	J/mol×K	779.38	Joback Method
cpg	959.87	J/mol×K	817.32	Joback Method
cpg	987.78	J/mol×K	855.27	Joback Method
cpg	1015.89	J/mol×K	893.21	Joback Method
cpg	1044.61	J/mol×K	931.16	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=R556871&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