C31 17A,21B,22S-Hopane

Inchi: InChI=1S/C31H54/c1-9-21(2)22-13-18-28(5)23(22)14-19-30(7)25(28)11-12-26-29(6)17-1
InchiKey: QFBGIDMRCNNMIW-KVIVRDSPSA-N
Formula: C31H54
SMILES: CCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C
Mol. weight [g/mol]: 426.76

Physical Properties

Property code	Value	Unit	Source
gf	372.85	kJ/mol	Joback Method
hf	-386.91	kJ/mol	Joback Method
hfus	24.46	kJ/mol	Joback Method
hvap	77.51	kJ/mol	Joback Method
log10ws	-9.61		Crippen Method
logp	9.524		Crippen Method
mcvol	393.350	ml/mol	McGowan Method
pc	903.97	kPa	Joback Method
rinpol	3229.00		NIST Webbook
rinpol	3229.00		NIST Webbook
tb	945.41	K	Joback Method
tc	1186.91	K	Joback Method
tf	591.01	K	Joback Method
vc	1.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1530.77	J/mol×K	945.41	Joback Method
cpg	1580.09	J/mol×K	985.66	Joback Method
cpg	1633.01	J/mol×K	1025.91	Joback Method
cpg	1690.31	J/mol×K	1066.16	Joback Method
cpg	1752.79	J/mol×K	1106.41	Joback Method
cpg	1821.23	J/mol×K	1146.66	Joback Method
cpg	1896.43	J/mol×K	1186.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R56286&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

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