11-methylsqualene

Inchi: InChI=1S/C31H52/c1-25(2)15-10-17-27(5)19-12-20-29(7)22-14-24-31(9)30(8)23-13-21-2
InchiKey: ONDJHVGPCYSWSC-PXFYGUSISA-N
Formula: C31H52
SMILES: CC(C)=CCCC(C)=CCCC(C)=CCCC(C)=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 424.74

Physical Properties

Property code	Value	Unit	Source
gf	631.61	kJ/mol	Joback Method
hf	-48.38	kJ/mol	Joback Method
hfus	68.09	kJ/mol	Joback Method
hvap	84.91	kJ/mol	Joback Method
log10ws	-11.92		Crippen Method
logp	10.995		Crippen Method
mcvol	421.850	ml/mol	McGowan Method
pc	675.70	kPa	Joback Method
rinpol	2830.00		NIST Webbook
rinpol	2830.00		NIST Webbook
tb	932.80	K	Joback Method
tc	1142.58	K	Joback Method
tf	310.93	K	Joback Method
vc	1.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1387.10	J/mol×K	932.80	Joback Method
cpg	1411.43	J/mol×K	967.76	Joback Method
cpg	1435.08	J/mol×K	1002.73	Joback Method
cpg	1458.22	J/mol×K	1037.69	Joback Method
cpg	1481.00	J/mol×K	1072.65	Joback Method
cpg	1503.59	J/mol×K	1107.62	Joback Method
cpg	1526.18	J/mol×K	1142.58	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R435922&Units=SI

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