phytadiene

Inchi: InChI=1S/C19H36/c1-16(2)10-7-12-18(5)14-9-15-19(6)13-8-11-17(3)4/h7,10,17-19H,1,8-
InchiKey: IVMZFGQGYPWKIO-JXMROGBWSA-N
Formula: C19H36
SMILES: C=C(C)C=CCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 264.49

Physical Properties

Property code	Value	Unit	Source
gf	261.29	kJ/mol	Joback Method
hf	-218.47	kJ/mol	Joback Method
hfus	32.01	kJ/mol	Joback Method
hvap	56.09	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.778		Crippen Method
mcvol	269.970	ml/mol	McGowan Method
pc	1173.63	kPa	Joback Method
rinpol	1861.00		NIST Webbook
rinpol	1861.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1856.00		NIST Webbook
tb	633.52	K	Joback Method
tc	808.28	K	Joback Method
tf	238.09	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.14	J/mol×K	633.52	Joback Method
cpg	760.02	J/mol×K	662.65	Joback Method
cpg	779.93	J/mol×K	691.77	Joback Method
cpg	798.91	J/mol×K	720.90	Joback Method
cpg	817.00	J/mol×K	750.02	Joback Method
cpg	834.24	J/mol×K	779.15	Joback Method

cpg	850.68	J/mol×K	808.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R216929&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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