phytadiene 2

Inchi: InChI=1S/C20H38/c1-7-18(4)12-9-14-20(6)16-10-15-19(5)13-8-11-17(2)3/h7,12,17,19-20
InchiKey: HNTNJYMWJHGCBD-LDADJPATSA-N
Formula: C20H38
SMILES: C=CC(C)=CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 278.52

Physical Properties

Property code	Value	Unit	Source
gf	269.71	kJ/mol	Joback Method
hf	-239.11	kJ/mol	Joback Method
hfus	34.60	kJ/mol	Joback Method
hvap	58.32	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	7.168		Crippen Method
mcvol	284.060	ml/mol	McGowan Method
pc	1100.08	kPa	Joback Method
rinpol	1871.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1984.00		NIST Webbook
tb	656.40	K	Joback Method
tc	830.57	K	Joback Method
tf	249.36	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.00	J/mol×K	656.40	Joback Method
cpg	818.15	J/mol×K	685.43	Joback Method
cpg	838.32	J/mol×K	714.46	Joback Method
cpg	857.55	J/mol×K	743.48	Joback Method
cpg	875.89	J/mol×K	772.51	Joback Method
cpg	893.37	J/mol×K	801.54	Joback Method
cpg	910.04	J/mol×K	830.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R221253&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume