phyt-2-ene

Inchi: InChI=1S/C19H38/c1-16(2)10-7-12-18(5)14-9-15-19(6)13-8-11-17(3)4/h10,17-19H,7-9,1
InchiKey: YJDOTLRMRJYGGN-UHFFFAOYSA-N
Formula: C19H38
SMILES: CC(C)=CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 266.50

Physical Properties

Property code	Value	Unit	Source
gf	173.45	kJ/mol	Joback Method
hf	-343.90	kJ/mol	Joback Method
hfus	33.29	kJ/mol	Joback Method
hvap	56.76	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	7.002		Crippen Method
mcvol	274.270	ml/mol	McGowan Method
pc	1140.57	kPa	Joback Method
rinpol	1853.00		NIST Webbook
rinpol	1811.00		NIST Webbook
ripol	1775.00		NIST Webbook
tb	636.84	K	Joback Method
tc	809.29	K	Joback Method
tf	239.85	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.11	J/mol×K	636.84	Joback Method
cpg	783.40	J/mol×K	665.58	Joback Method
cpg	803.73	J/mol×K	694.32	Joback Method
cpg	823.14	J/mol×K	723.07	Joback Method
cpg	841.67	J/mol×K	751.81	Joback Method
cpg	859.34	J/mol×K	780.55	Joback Method
cpg	876.21	J/mol×K	809.29	Joback Method

Sources

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=R216909&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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