cis-Phytol

Other names: (Z)-Phytol
Inchi: InChI=1S/C20H40O/c1-17(2)9-6-10-18(3)11-7-12-19(4)13-8-14-20(5)15-16-21/h15,17-19
InchiKey: BOTWFXYSPFMFNR-ITKMZDMZSA-N
Formula: C20H40O
SMILES: CC(=CCO)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 296.53

Physical Properties

Property code	Value	Unit	Source
gf	45.05	kJ/mol	Joback Method
hf	-516.77	kJ/mol	Joback Method
hfus	39.97	kJ/mol	Joback Method
hvap	75.67	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	6.364		Crippen Method
mcvol	294.230	ml/mol	McGowan Method
pc	1137.50	kPa	Joback Method
rinpol	2086.00		NIST Webbook
rinpol	2114.00		NIST Webbook
rinpol	2113.00		NIST Webbook
rinpol	2114.00		NIST Webbook
rinpol	2114.00		NIST Webbook
rinpol	2112.00		NIST Webbook
rinpol	2114.00		NIST Webbook
rinpol	2113.00		NIST Webbook
rinpol	2113.00		NIST Webbook
rinpol	2112.00		NIST Webbook
rinpol	2114.00		NIST Webbook
rinpol	2086.00		NIST Webbook
ripol	2570.00		NIST Webbook
ripol	2555.00		NIST Webbook
ripol	2570.00		NIST Webbook
ripol	2573.00		NIST Webbook
ripol	2555.00		NIST Webbook
ripol	2570.00		NIST Webbook
tb	751.90	K	Joback Method
tc	926.94	K	Joback Method

tf	311.94	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.37	J/mol×K	751.90	Joback Method
cpg	923.39	J/mol×K	781.07	Joback Method
cpg	941.52	J/mol×K	810.25	Joback Method
cpg	958.79	J/mol×K	839.42	Joback Method
cpg	975.26	J/mol×K	868.59	Joback Method
cpg	990.97	J/mol×K	897.76	Joback Method
cpg	1005.95	J/mol×K	926.94	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R290467&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