

Phytol

Other names:	2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]-trans-Phytol 3,7,11,15-Tetramethyl-2-hexadecen-1-ol-, (2E,7R,11R)- (2E,7R,11R)-3,7,11,15-Tetramethyl-2-hexadecen-1-ol 3,7,11,15-teramethyl-2-hexadecene-1-ol-, (2E,7R,11R)-(E)-Phytol 3,7,11,15-Tetramethyl-2-hexadecen-1-ol 3,7,11,15-teramethyl-2-hexadecene-1-ol 3,7,11,15-tetramethylhexadec-2-en-1-ol
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:	BOTWFXYSPPFMFNR-PFIWFTBQSA-N
Formula:	C20H40O
SMILES:	CC(=CCO)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]:	296.53
CAS:	150-86-7

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	2090.00		NIST Webbook
rinpol	2128.00		NIST Webbook
rinpol	2145.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2115.60		NIST Webbook
rinpol	2119.80		NIST Webbook
rinpol	2119.00		NIST Webbook
rinpol	2113.90		NIST Webbook
rinpol	2080.00		NIST Webbook
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rinpol	2105.00		NIST Webbook

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rinpol	2108.00	NIST Webbook
rinpol	2118.00	NIST Webbook
rinpol	2076.00	NIST Webbook
rinpol	2100.00	NIST Webbook
rinpol	2100.00	NIST Webbook
rinpol	2089.00	NIST Webbook
rinpol	2135.00	NIST Webbook
rinpol	2114.00	NIST Webbook
rinpol	2087.00	NIST Webbook
rinpol	2110.00	NIST Webbook
rinpol	2083.00	NIST Webbook
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ripol	2599.00		NIST Webbook
ripol	2622.00		NIST Webbook
ripol	2604.00		NIST Webbook
ripol	2622.00		NIST Webbook
tb	751.90	K	Joback Method
tc	926.94	K	Joback Method
tf	311.94	K	Joback Method
vc	1.137	m ³ /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

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=C150867&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
rlnpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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