

1,6,10,14-Hexadecatetraen-3-ol, 3,7,11,15-tetramethyl-, (E,E)-

Other names:

Geranyl linalol

Geranyllinalool

Linalool, geranyl-

(E,E)-Geranyllinalool

Geranyllinalol

(E,E)-3,7,11,15-tetramethylhexadeca-1,6,10,14-tetraen-3-ol

Inchi:

InChI=1S/C20H34O/c1-7-20(6,21)16-10-15-19(5)14-9-13-18(4)12-8-11-17(2)3/h7,11,13,15,19

InchiKey:

IQDXAJNQKSIPGB-HQSZA HFGSA-N

Formula:

C₂₀H₃₄O

SMILES:

C=CC(C)(O)CCC=C(C)CCC=C(C)CCC=C(C)C

Mol. weight [g/mol]:

290.48

CAS:

1113-21-9

Physical Properties

Property code	Value	Unit	Source
gf	286.39	kJ/mol	Joback Method
hf	-169.39	kJ/mol	Joback Method
hfus	39.63	kJ/mol	Joback Method
hvap	74.94	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	6.123		Crippen Method
mcvol	281.330	ml/mol	McGowan Method
pc	1262.85	kPa	Joback Method
rinpol	2008.00		NIST Webbook
rinpol	2034.00		NIST Webbook
rinpol	2034.00		NIST Webbook
rinpol	2031.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2020.00		NIST Webbook
rinpol	2020.00		NIST Webbook
rinpol	2020.00		NIST Webbook
ripol	2559.00		NIST Webbook
ripol	2522.00		NIST Webbook
ripol	2537.00		NIST Webbook
ripol	2551.00		NIST Webbook
ripol	2551.00		NIST Webbook
ripol	2551.00		NIST Webbook

ripol	2551.00		NIST Webbook
ripol	2551.00		NIST Webbook
ripol	2559.00		NIST Webbook
ripol	2551.00		NIST Webbook
ripol	2522.00		NIST Webbook
ripol	2491.00		NIST Webbook
ripol	2492.00		NIST Webbook
ripol	2491.00		NIST Webbook
tb	754.75	K	Joback Method
tc	940.55	K	Joback Method
tf	319.52	K	Joback Method
vc	1.087	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.45	J/mol×K	754.75	Joback Method
cpg	847.86	J/mol×K	785.72	Joback Method
cpg	864.44	J/mol×K	816.68	Joback Method
cpg	880.28	J/mol×K	847.65	Joback Method
cpg	895.46	J/mol×K	878.62	Joback Method
cpg	910.07	J/mol×K	909.59	Joback Method
cpg	924.18	J/mol×K	940.55	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=C1113219&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.cheméo.com/cid/64-323-2/1-6-10-14-Hexadecatetraen-3-ol-3-7-11-15-tetramethyl-E-E.pdf>

Generated by Cheméo on 2024-04-20 10:54:08.147233315 +0000 UTC m=+15899697.067810631.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.