Isophytol

Other names:	1-Hexadecen-3-ol, 3,7,11,15-tetramethyl-
	Hexadec-1-en-3-ol, 3,7,11,15-tetramethyl-
	1-Hexadecene-3-ol, 3,7,11,15-tetramethyl
	NSC 93744
	3,7,11,15-Tetramethylhexadec-1-en-3-ol
	2,6,10,14-Tetramethylhexadec-15-en-14-ol
	3,7,11,15-Tetramethyl-1-hexadecen-3-ol
Inchi:	InChI=1S/C20H40O/c1-7-20(6,21)16-10-15-19(5)14-9-13-18(4)12-8-11-17(2)3/h7,17-19,2
InchiKey:	KEVYVLWNCKMXJX-UHFFFAOYSA-N
Formula:	C20H40O
SMILES:	C=CC(C)(O)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]:	296.53
CAS:	505-32-8

Physical Properties

Property code	Value	Unit	Source
gf	64.06	kJ/mol	Joback Method
hf	-507.52	kJ/mol	Joback Method
hfus	32.38	kJ/mol	Joback Method
hvap	73.66	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	6.362		Crippen Method
mcvol	294.230	ml/mol	McGowan Method
pc	1140.57	kPa	Joback Method
rinpol	1951.00		NIST Webbook
rinpol	1948.60		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1938.00		NIST Webbook
rinpol	1943.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1943.00		NIST Webbook
rinpol	1956.00		NIST Webbook

rinpol	1949.00	NIST Webbook
rinpol	1946.00	NIST Webbook
rinpol	1940.00	NIST Webbook
rinpol	1949.00	NIST Webbook
rinpol	1950.00	NIST Webbook
rinpol	1950.00	NIST Webbook
rinpol	1938.00	NIST Webbook
rinpol	1954.00	NIST Webbook
rinpol	1945.00	NIST Webbook
rinpol	1943.00	NIST Webbook
rinpol	1922.00	NIST Webbook
rinpol	1947.00	NIST Webbook
rinpol	1948.00	NIST Webbook
rinpol	1950.00	NIST Webbook
rinpol	1945.00	NIST Webbook
rinpol	1932.00	NIST Webbook
rinpol	1945.00	NIST Webbook
rinpol	1946.00	NIST Webbook
rinpol	1944.00	NIST Webbook
rinpol	1949.00	NIST Webbook
rinpol	1950.00	NIST Webbook
rinpol	1950.00	NIST Webbook
rinpol	1945.00	NIST Webbook
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rinpol	1950.00	NIST Webbook
rinpol	1947.00	NIST Webbook
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rinpol	1948.00	NIST Webbook
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rinpol	1943.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1922.00		NIST Webbook
rinpol	1932.00		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1942.00		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1944.00		NIST Webbook
rinpol	1956.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1942.00		NIST Webbook
rinpol	1938.00		NIST Webbook
rinpol	1938.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2296.00		NIST Webbook
ripol	2299.00		NIST Webbook
ripol	2296.00		NIST Webbook
ripol	2282.00		NIST Webbook
ripol	2327.00		NIST Webbook
ripol	2282.00		NIST Webbook
ripol	2286.00		NIST Webbook
ripol	2278.00		NIST Webbook
ripol	2296.00		NIST Webbook
ripol	2296.00		NIST Webbook
tb	741.31	K	Joback Method
tc	916.20	K	Joback Method
tf	331.64	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	903.98	J/mol×K	741.31	Joback Method
cpg	923.04	J/mol×K	770.46	Joback Method
cpg	941.17	J/mol×K	799.61	Joback Method
cpg	958.41	J/mol×K	828.75	Joback Method
cpg	974.81	J/mol×K	857.90	Joback Method
cpg	990.43	J/mol×K	887.05	Joback Method
cpg	1005.31	J/mol×K	916.20	Joback Method
dvisc	0.0150671	Pa×s	331.64	Joback Method
dvisc	0.0017320	Pa×s	399.92	Joback Method
dvisc	0.0003742	Pa×s	468.20	Joback Method
dvisc	0.0001194	Pa×s	536.47	Joback Method
dvisc	0.0000493	Pa×s	604.75	Joback Method
dvisc	0.0000244	Pa×s	673.03	Joback Method
dvisc	0.0000137	Pa×s	741.31	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C505328&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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