

3-Hexadecanol, 3,7,11,15-tetramethyl-

Other names:	3,7,11,15-tetramethylhexadecan-3-ol
Inchi:	InChI=1S/C20H42O/c1-7-20(6,21)16-10-15-19(5)14-9-13-18(4)12-8-11-17(2)3/h17-19,21
InchiKey:	CVPIIXFZNPKANT-UHFFFAOYSA-N
Formula:	C20H42O
SMILES:	CCC(C)(O)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]:	298.55
CAS:	85761-30-4

Physical Properties

Property code	Value	Unit	Source
gf	-23.78	kJ/mol	Joback Method
hf	-632.95	kJ/mol	Joback Method
hfus	33.66	kJ/mol	Joback Method
hvap	74.33	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.587		Crippen Method
mcvol	298.530	ml/mol	McGowan Method
pc	1108.89	kPa	Joback Method
rinpol	1974.00		NIST Webbook
rinpol	1974.00		NIST Webbook
ripol	2190.00		NIST Webbook
ripol	2190.00		NIST Webbook
tb	744.63	K	Joback Method
tc	918.64	K	Joback Method
tf	333.40	K	Joback Method
vc	1.145	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.61	J/mol×K	744.63	Joback Method
cpg	949.19	J/mol×K	773.63	Joback Method
cpg	967.81	J/mol×K	802.63	Joback Method
cpg	985.54	J/mol×K	831.63	Joback Method

cpg	1002.40	J/mol×K	860.63	Joback Method
cpg	1018.45	J/mol×K	889.64	Joback Method
cpg	1033.74	J/mol×K	918.64	Joback Method
dvisc	0.0150419	Paxs	333.40	Joback Method
dvisc	0.0016961	Paxs	401.94	Joback Method
dvisc	0.0003612	Paxs	470.48	Joback Method
dvisc	0.0001140	Paxs	539.01	Joback Method
dvisc	0.0000467	Paxs	607.55	Joback Method
dvisc	0.0000229	Paxs	676.09	Joback Method
dvisc	0.0000128	Paxs	744.63	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=C85761304&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
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

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