

3-Hexanol, 2,2,5,5-tetramethyl-

Inchi:	InChI=1S/C10H22O/c1-9(2,3)7-8(11)10(4,5)6/h8,11H,7H2,1-6H3
InchiKey:	CFEYPBVKHMCZCFR-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CC(C)(C)CC(O)C(C)(C)C
Mol. weight [g/mol]:	158.28
CAS:	55073-86-4

Physical Properties

Property code	Value	Unit	Source
gf	-100.26	kJ/mol	Joback Method
hf	-424.74	kJ/mol	Joback Method
hfus	7.39	kJ/mol	Joback Method
hvap	51.55	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.830		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
tb	446.65 ± 4.00	K	NIST Webbook
tb	443.15 ± 5.00	K	NIST Webbook
tc	692.84	K	Joback Method
tf	253.12	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.67	J/mol×K	513.48	Joback Method
cpg	455.72	J/mol×K	662.94	Joback Method
cpg	443.43	J/mol×K	633.05	Joback Method
cpg	430.42	J/mol×K	603.16	Joback Method
cpg	416.65	J/mol×K	573.27	Joback Method
cpg	402.08	J/mol×K	543.37	Joback Method
cpg	467.33	J/mol×K	692.84	Joback Method
dvisc	0.0001107	Pa×s	513.48	Joback Method

dvisc	0.0002073	Pa×s	470.09	Joback Method
dvisc	0.0004411	Pa×s	426.69	Joback Method
dvisc	0.0011137	Pa×s	383.30	Joback Method
dvisc	0.0035617	Pa×s	339.91	Joback Method
dvisc	0.0160077	Pa×s	296.51	Joback Method
dvisc	0.1204426	Pa×s	253.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55073864&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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