

3-Methyl-1-hexen-3-ol

Other names:	1-Hexen-3-ol, 3-methyl-3-Methyl-hexen-(1)-ol-(3)
Inchi:	InChI=1S/C7H14O/c1-4-6-7(3,8)5-2/h5,8H,2,4,6H2,1,3H3
InchiKey:	JNLMZYGDTPRAMM-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	C=CC(C)(O)CCC
Mol. weight [g/mol]:	114.19
CAS:	55145-28-3

Physical Properties

Property code	Value	Unit	Source
gf	-38.08	kJ/mol	Joback Method
hf	-223.36	kJ/mol	Joback Method
hfus	9.28	kJ/mol	Joback Method
hvap	45.89	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.723		Crippen Method
mvol	111.060	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
tb	405.15 ± 3.00	K	NIST Webbook
tc	618.51	K	Joback Method
tf	230.13	K	Joback Method
vc	0.416	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.09	J/mol×K	445.19	Joback Method
cpg	245.12	J/mol×K	474.08	Joback Method
cpg	255.60	J/mol×K	502.96	Joback Method
cpg	265.53	J/mol×K	531.85	Joback Method
cpg	274.94	J/mol×K	560.74	Joback Method
cpg	283.87	J/mol×K	589.63	Joback Method
cpg	292.33	J/mol×K	618.51	Joback Method

dvisc	0.0922078	Paxs	230.13	Joback Method
dvisc	0.0172289	Paxs	265.97	Joback Method
dvisc	0.0047949	Paxs	301.82	Joback Method
dvisc	0.0017508	Paxs	337.66	Joback Method
dvisc	0.0007757	Paxs	373.50	Joback Method
dvisc	0.0003963	Paxs	409.35	Joback Method
dvisc	0.0002256	Paxs	445.19	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=C55145283&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvac:	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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