

3-Methyl-3-hexen-2-ol

Inchi:	InChI=1S/C7H14O/c1-4-5-6(2)7(3)8/h5,7-8H,4H2,1-3H3/b6-5+
InchiKey:	ALSBKNSBCLYOOI-AATRIKPKSA-N
Formula:	C7H14O
SMILES:	CCC=C(C)C(C)O
Mol. weight [g/mol]:	114.19
CAS:	76966-27-3

Physical Properties

Property code	Value	Unit	Source
gf	-59.53	kJ/mol	Joback Method
hf	-237.89	kJ/mol	Joback Method
hfus	13.34	kJ/mol	Joback Method
hvap	47.50	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.723		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
tb	455.34	K	Joback Method
tc	629.75	K	Joback Method
tf	195.43	K	Joback Method
vc	0.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.54	J/mol×K	455.34	Joback Method
cpg	242.22	J/mol×K	484.41	Joback Method
cpg	252.41	J/mol×K	513.48	Joback Method
cpg	262.13	J/mol×K	542.55	Joback Method
cpg	271.41	J/mol×K	571.61	Joback Method
cpg	280.26	J/mol×K	600.68	Joback Method
cpg	288.70	J/mol×K	629.75	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41344e+01
Coeff. B	-3.71692e+03
Coeff. C	-6.12880e+01
Temperature range (K), min.	329.72
Temperature range (K), max.	482.57

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C76966273&Units=SI

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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