3-Hexanol, 3-methyl-

Other names:	2-Ethyl-2-pentanol
	3-Methyl-3-hexanol
	3-Methyl-hexanol-(3)
	3-methylhexan-3-ol
Inchi:	InChI=1S/C7H16O/c1-4-6-7(3,8)5-2/h8H,4-6H2,1-3H3
InchiKey:	KYWJZCSJMOILIZ-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCC(C)(O)CC
Mol. weight [g/mol]:	116.20
CAS:	597-96-6

Physical Properties

Property code	Value	Unit	Source
gf	-125.92	kJ/mol	Joback Method
hf	-348.79	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	46.56	kJ/mol	Joback Method
log10ws	-0.98		Estimated Solubility Method
log10ws	-1.00		Aqueous Solubility Prediction Method
logp	1.948		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
rinpol	827.00		NIST Webbook
rinpol	827.00		NIST Webbook
tb	413.15 ± 3.00	K	NIST Webbook
tb	415.65 ± 3.00	K	NIST Webbook
tb	416.15 ± 3.00	K	NIST Webbook
tb	412.65 ± 3.00	K	NIST Webbook
tb	413.15 ± 3.00	K	NIST Webbook
tb	411.15 ± 3.00	K	NIST Webbook
tb	413.65 ± 3.00	K	NIST Webbook
tb	415.95 ± 0.50	K	NIST Webbook
tb	413.65 ± 3.00	K	NIST Webbook
tb	415.95 ± 1.00	K	NIST Webbook
tc	618.48	K	Joback Method
tf	231.89	K	Joback Method

vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.34	J/mol×K	618.48	Joback Method
cpg	303.23	J/mol×K	590.15	Joback Method
cpg	293.67	J/mol×K	561.82	Joback Method
cpg	283.62	J/mol×K	533.50	Joback Method
cpg	273.08	J/mol×K	505.17	Joback Method
cpg	262.01	J/mol×K	476.84	Joback Method
cpg	250.39	J/mol×K	448.51	Joback Method
dvisc	0.0985996	Pa×s	231.89	Joback Method
dvisc	0.0002207	Pa×s	448.51	Joback Method
dvisc	0.0003910	Pa×s	412.41	Joback Method
dvisc	0.0007730	Pa×s	376.30	Joback Method
dvisc	0.0017661	Pa×s	340.20	Joback Method
dvisc	0.0049095	Pa×s	304.10	Joback Method
dvisc	0.0179763	Pa×s	267.99	Joback Method
hvapt	53.60	kJ/mol	369.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57516e+01
Coeff. B	-3.78938e+03
Coeff. C	-7.36330e+01
Temperature range (K), min.	318.68
Temperature range (K), max.	436.60

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/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C597966&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume