3-Methyloctanol

Other names: 3-methyl-1-octanol
Inchi: InChI=1S/C9H20O/c1-3-4-5-6-9(2)7-8-10/h9-10H,3-8H2,1-2H3
InchiKey: CLFSZAMBOZSCOS-UHFFFAOYSA-N
Formula: C9H20O
SMILES: CCCCCC(C)CCO
Mol. weight [g/mol]: 144.25
CAS: 38514-02-2

Physical Properties

Property code	Value	Unit	Source
gf	-114.36	kJ/mol	Joback Method
hf	-386.60	kJ/mol	Joback Method
hfus	19.63	kJ/mol	Joback Method
hvap	51.92	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.585		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1135.00		NIST Webbook
rinpol	1135.00		NIST Webbook
tb	497.06	K	Joback Method
tc	659.14	K	Joback Method
tf	237.01	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.58	J/mol×K	497.06	Joback Method
cpg	347.30	J/mol×K	524.07	Joback Method
cpg	359.54	J/mol×K	551.09	Joback Method
cpg	371.30	J/mol×K	578.10	Joback Method
cpg	382.60	J/mol×K	605.11	Joback Method
cpg	393.45	J/mol×K	632.13	Joback Method

cpg	403.87	J/mol×K	659.14	Joback Method
dvisc	0.0878509	Pa×s	237.01	Joback Method
dvisc	0.0131188	Pa×s	280.35	Joback Method
dvisc	0.0032599	Pa×s	323.69	Joback Method
dvisc	0.0011254	Pa×s	367.03	Joback Method
dvisc	0.0004864	Pa×s	410.38	Joback Method
dvisc	0.0002468	Pa×s	453.72	Joback Method
dvisc	0.0001409	Pa×s	497.06	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.72143e+01
Coeff. B	-4.95540e+03
Coeff. C	-7.26440e+01
Temperature range (K), min.	365.40
Temperature range (K), max.	488.96

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=C38514022&Units=SI
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
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume