1,7-Octanediol, 3,7-dimethyl-

Other names:	1,2-Octandiol, 3,7-dimethyl-
	1,2-Octanediol, 3,7-dimethyl-
	1-Octanol, 3,7-dimethyl-7-hydroxy-
	2,8-Octanediol, 2,6-dimethyl-
	3,7-Dimethyl-1,7-octanediol
	3,7-dimethyloctane-1,7-diol
	7-Hydroxy-3,7-dimethyloctan-1-ol
	7-Hydroxy-6,7-dihydrocitronellol
	Citronellol hydrate
	Citronellol, hydroxy-
	NSC 406140
	Octane-1,7-diol, 3,7-dimethyl
Inchi:	InChI=1S/C10H22O2/c1-9(6-8-11)5-4-7-10(2,3)12/h9,11-12H,4-8H2,1-3H3
InchiKey:	FPCCDPXRNNVUOM-UHFFFAOYSA-N
Formula:	C10H22O2
SMILES:	CC(CCO)CCCC(C)(C)O
Mol. weight [g/mol]:	174.28
CAS:	107-74-4

Physical Properties

Property code	Value	Unit	Source
gf	-239.92	kJ/mol	Joback Method
hf	-568.22	kJ/mol	Joback Method
hfus	18.89	kJ/mol	Joback Method
hvap	69.53	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	1.946		Crippen Method
mcvol	163.500	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
tb	608.89	K	Joback Method
tc	774.28	K	Joback Method
tf	311.52	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.21	J/mol×K	608.89	Joback Method
cpg	457.43	J/mol×K	636.46	Joback Method
cpg	469.08	J/mol×K	664.02	Joback Method
cpg	480.18	J/mol×K	691.59	Joback Method
cpg	490.76	J/mol×K	719.15	Joback Method
cpg	500.85	J/mol×K	746.72	Joback Method
cpg	510.46	J/mol×K	774.28	Joback Method
dvisc	0.0572327	Pa×s	311.52	Joback Method
dvisc	0.0064076	Pa×s	361.08	Joback Method
dvisc	0.0012170	Pa×s	410.64	Joback Method
dvisc	0.0003306	Pa×s	460.20	Joback Method
dvisc	0.0001157	Pa×s	509.77	Joback Method
dvisc	0.0000488	Pa×s	559.33	Joback Method
dvisc	0.0000237	Pa×s	608.89	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.77056e+01
Coeff. B	-5.69159e+03
Coeff. C	-9.07560e+01
Temperature range (K), min.	417.52
Temperature range (K), max.	549.97

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C107744&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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume