1-Octanol, 2,2-dimethyl-

Other names:	2,2-Dimethyl-1-octanol
	2,2-Dimethyl-1-octanol; 2,2-Dimethyloctanol
	2,2-Dimethyloctanol
Inchi:	InChI=1S/C10H22O/c1-4-5-6-7-8-10(2,3)9-11/h11H,4-9H2,1-3H3
InchiKey:	KEXGXAGJHHCTKD-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CCCCCCC(C)(C)CO
Mol. weight [g/mol]:	158.28
CAS:	2370-14-1

Physical Properties

Property code	Value	Unit	Source
gf	-100.66	kJ/mol	Joback Method
hf	-410.71	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	53.24	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.975		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
tb	481.15 ± 3.00	K	NIST Webbook
tc	683.80	K	Joback Method
tf	265.70	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.55	J/mol×K	517.15	Joback Method
cpg	397.63	J/mol×K	544.92	Joback Method
cpg	411.07	J/mol×K	572.70	Joback Method
cpg	423.89	J/mol×K	600.47	Joback Method
cpg	436.13	J/mol×K	628.25	Joback Method
cpg	447.81	J/mol×K	656.02	Joback Method

cpg	458.94	J/mol×K	683.80	Joback Method
dvisc	0.0428890	Pa×s	265.70	Joback Method
dvisc	0.0082611	Pa×s	307.61	Joback Method
dvisc	0.0023619	Pa×s	349.52	Joback Method
dvisc	0.0008829	Pa×s	391.43	Joback Method
dvisc	0.0003993	Pa×s	433.33	Joback Method
dvisc	0.0002077	Pa×s	475.24	Joback Method
dvisc	0.0001201	Pa×s	517.15	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63942e+01
Coeff. B	-4.78381e+03
Coeff. C	-7.49100e+01
Temperature range (K), min.	371.92
Temperature range (K), max.	506.56

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
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=C2370141&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
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