

1-Octanol, 3,7-dimethyl-

Other names:	Citronellol, dihydro- Dihydrocitronellol Geraniol tetrahydride Geraniol, perhydro- Geraniol, tetrahydro- Pelargol Perhydrogeraniol Tetrahydrogeraniol 2,6-Dimethyl-8-octanol 3,7-Dimethyl-1-octanol 3,7-Dimethyloctan-1-ol Dimethyloctanol NSC 18917 DL-3,7-dimethyl-1-octanol
Inchi:	InChI=1S/C10H22O/c1-9(2)5-4-6-10(3)7-8-11/h9-11H,4-8H2,1-3H3
InchiKey:	PRNCMAKCNVRZFX-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CC(C)CCCC(C)CCO
Mol. weight [g/mol]:	158.28
CAS:	59204-02-3

Physical Properties

Property code	Value	Unit	Source
gf	-108.38	kJ/mol	Joback Method
hf	-412.52	kJ/mol	Joback Method
hfus	18.70	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.831		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
tb	485.65 ± 4.00	K	NIST Webbook
tc	683.75	K	Joback Method
tf	233.28	K	Joback Method
vc	0.603	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.07	J/molxK	519.50	Joback Method
cpg	444.88	J/molxK	656.37	Joback Method
cpg	433.16	J/molxK	629.00	Joback Method
cpg	420.93	J/molxK	601.62	Joback Method
cpg	408.18	J/molxK	574.25	Joback Method
cpg	394.90	J/molxK	546.87	Joback Method
cpg	456.11	J/molxK	683.75	Joback Method
dvisc	0.0001109	Paxs	519.50	Joback Method
dvisc	0.0002007	Paxs	471.80	Joback Method
dvisc	0.0004150	Paxs	424.09	Joback Method
dvisc	0.0010317	Paxs	376.39	Joback Method
dvisc	0.0033408	Paxs	328.69	Joback Method
dvisc	0.0161218	Paxs	280.98	Joback Method
dvisc	0.1480969	Paxs	233.28	Joback Method

Sources

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=C59204023&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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