

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
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:	106-21-8

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
rinpol	1180.70		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1180.60		NIST Webbook
rinpol	1181.60		NIST Webbook
rinpol	1181.60		NIST Webbook
rinpol	1186.00		NIST Webbook

rinpol	1183.30		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1196.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1664.80		NIST Webbook
ripol	1666.40		NIST Webbook
ripol	1666.30		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1666.40		NIST Webbook
tb	519.50	K	Joback Method
tc	683.75	K	Joback Method
tf	233.28	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.07	J/mol×K	519.50	Joback Method
cpg	394.90	J/mol×K	546.87	Joback Method
cpg	408.18	J/mol×K	574.25	Joback Method
cpg	420.93	J/mol×K	601.62	Joback Method
cpg	433.16	J/mol×K	629.00	Joback Method
cpg	444.88	J/mol×K	656.37	Joback Method
cpg	456.11	J/mol×K	683.75	Joback Method
cpl	367.21	J/mol×K	298.15	NIST Webbook
dvisc	0.1480969	Pa×s	233.28	Joback Method
dvisc	0.0161218	Pa×s	280.98	Joback Method
dvisc	0.0033408	Pa×s	328.69	Joback Method
dvisc	0.0010317	Pa×s	376.39	Joback Method
dvisc	0.0004150	Pa×s	424.09	Joback Method
dvisc	0.0002007	Pa×s	471.80	Joback Method
dvisc	0.0001109	Pa×s	519.50	Joback Method
hvapt	79.10	kJ/mol	404.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.70	K	1.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106218&Units=SI
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
cpl:	Liquid phase 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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