2-Octanol, 8,8-dimethoxy-2,6-dimethyl-

Other names:	Octanal, 7-hydroxy-3,7-dimethyl-, dimethyl acetal
	Hydroxycitronellal dimethyl acetal
	Laurine dimethyl acetal
	7-Hydroxy-3,7-dimethyloctanal, dimethyl acetal
	Citronellal hydrate dimethylacetal
	Hydroxycitronellal DMA
	8,8-Dimethoxy-2,6-dimethyl-2-octanol
	1,1-Dimethoxy-3,7-dimethyl-7-octanol
	NSC 76412
	8,8-dimethoxy-2,6-dimethyloctan-2-ol
Inchi:	InChI=1S/C12H26O3/c1-10(9-11(14-4)15-5)7-6-8-12(2,3)13/h10-11,13H,6-9H2,1-5H3
InchiKey:	QCJVKUULZGKQDG-UHFFFAOYSA-N
Formula:	C12H26O3
SMILES:	COC(CC(C)CCCC(C)(C)O)OC
Mol. weight [g/mol]:	218.33
CAS:	141-92-4

Physical Properties

Property code	Value	Unit	Source
gf	-298.70	kJ/mol	Joback Method
hf	-726.99	kJ/mol	Joback Method
hfus	18.84	kJ/mol	Joback Method
hvap	61.73	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.573		Crippen Method
mcvol	197.550	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	1413.70		NIST Webbook
tb	606.87	K	Joback Method
tc	777.03	K	Joback Method
tf	302.70	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.30	J/mol×K	606.87	Joback Method
cpg	553.71	J/mol×K	635.23	Joback Method
cpg	568.44	J/mol×K	663.59	Joback Method
cpg	582.51	J/mol×K	691.95	Joback Method
cpg	595.94	J/mol×K	720.31	Joback Method
cpg	608.73	J/mol×K	748.67	Joback Method
cpg	620.90	J/mol×K	777.03	Joback Method
dvisc	0.0171709	Pa×s	302.70	Joback Method
dvisc	0.0029451	Pa×s	353.39	Joback Method
dvisc	0.0007862	Pa×s	404.09	Joback Method
dvisc	0.0002817	Pa×s	454.78	Joback Method
dvisc	0.0001240	Pa×s	505.48	Joback Method
dvisc	0.0000634	Pa×s	556.17	Joback Method
dvisc	0.0000363	Pa×s	606.87	Joback Method

Sources

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=C141924&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume