

7-Octene-2,6-diol, 2,6-dimethyl-

Other names:	6,7-Dihydro-7-hydroxylinalool 3,7-Dimethyloct-1-ene-3,7-diol 2,6-Dimethyl-7-octene-2,6-diol 1-Octen-3,7-diol, 3,7-dimethyl 2,6-Dimethyl-7-octen-2,6-diol 2,6-Dimethyloct-7-en-2,6-diol 3,7-Dimethyl-3,7-dihydroxyoct-1-ene 7-Hydroxy-6,7-dihydrolinalool linalool hydrate 3,7-Dimethyl-1-octen-3,7-diol 3,7-dimethyl-1-octene-3,7-diol 2,6-dimethyloct-7-ene-2,6-diol
Inchi:	InChI=1S/C10H20O2/c1-5-10(4,12)8-6-7-9(2,3)11/h5,11-12H,1,6-8H2,2-4H3
InchiKey:	SRPFYGUVQUDURC-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	C=CC(C)(O)CCCC(C)(C)O
Mol. weight [g/mol]:	172.26
CAS:	29210-77-3

Physical Properties

Property code	Value	Unit	Source
gf	-146.80	kJ/mol	Joback Method
hf	-446.26	kJ/mol	Joback Method
hfus	13.72	kJ/mol	Joback Method
hvap	67.95	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.865		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1237.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1983.00		NIST Webbook
ripol	1935.00		NIST Webbook
ripol	1982.00		NIST Webbook
ripol	1981.00		NIST Webbook
ripol	1981.00		NIST Webbook
ripol	1993.00		NIST Webbook

ripol	1959.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	1996.00		NIST Webbook
ripol	1993.00		NIST Webbook
tb	602.78	K	Joback Method
tc	775.06	K	Joback Method
tf	327.18	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.94	J/mol×K	602.78	Joback Method
cpg	438.82	J/mol×K	631.49	Joback Method
cpg	450.05	J/mol×K	660.21	Joback Method
cpg	460.65	J/mol×K	688.92	Joback Method
cpg	470.67	J/mol×K	717.63	Joback Method
cpg	480.15	J/mol×K	746.35	Joback Method
cpg	489.14	J/mol×K	775.06	Joback Method
dvisc	0.0308575	Pa×s	327.18	Joback Method
dvisc	0.0045164	Pa×s	373.11	Joback Method
dvisc	0.0010074	Pa×s	419.05	Joback Method
dvisc	0.0003022	Pa×s	464.98	Joback Method
dvisc	0.0001126	Pa×s	510.91	Joback Method
dvisc	0.0000494	Pa×s	556.85	Joback Method
dvisc	0.0000245	Pa×s	602.78	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=C29210773&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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