

2,7-Octadiene-1,6-diol, 2,6-dimethyl-, (E)-

Other names:	2,6-dimethyl-2(E),7-octadiene-1,6-diol (E)-2,6-Dimethyl-2,7-octadien-1,6-diol (E)-2,6-dimethyl-2,7-octadiene-1,6-diol (E)-2,6-Dimethyl-octa-2,7-dien-1,6-diol (E)-2,6-dimethylocta-2,7-diene-1,6-diol (E)-2,6-Dimethyl-octa-2.7-dien-1,6-diol E-8-Hydroxylinalol (E)-8-hydroxylinalool trans-8-hydroxylinalool (trans-3,7-dimethyl-1,6-octadiene-3,8-diol) trans-2,6-Dimethyl-2,7-octadien-1,6-diol trans-2,6-dimethyl-2,7-octadiene-1,6-diol
Inchi:	InChI=1S/C10H18O2/c1-4-10(3,12)7-5-6-9(2)8-11/h4,6,11-12H,1,5,7-8H2,2-3H3/b9-6+
InchiKey:	NSMIMJYEKVSYMT-RMKNXTFCSA-N
Formula:	C10H18O2
SMILES:	C=CC(C)(O)CCC=C(C)CO
Mol. weight [g/mol]:	170.25
CAS:	75991-61-6

Physical Properties

Property code	Value	Unit	Source
gf	-77.97	kJ/mol	Joback Method
hf	-330.08	kJ/mol	Joback Method
hfus	20.03	kJ/mol	Joback Method
hvap	69.28	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.642		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	1333.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1339.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1342.00		NIST Webbook

ripol	1345.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	2266.00		NIST Webbook
ripol	2275.00		NIST Webbook
ripol	2298.00		NIST Webbook
ripol	2294.00		NIST Webbook
ripol	2296.00		NIST Webbook
ripol	2294.00		NIST Webbook
ripol	2281.00		NIST Webbook
ripol	2267.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2282.00		NIST Webbook
ripol	2270.00		NIST Webbook
ripol	2254.00		NIST Webbook
ripol	2277.00		NIST Webbook
ripol	2297.00		NIST Webbook
ripol	2294.00		NIST Webbook
ripol	2294.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2294.00		NIST Webbook
ripol	2290.00		NIST Webbook
ripol	2260.00		NIST Webbook
ripol	2294.00		NIST Webbook
ripol	2272.00		NIST Webbook
ripol	2270.00		NIST Webbook
ripol	2275.00		NIST Webbook
ripol	2285.00		NIST Webbook
ripol	2267.00		NIST Webbook
ripol	2318.00		NIST Webbook
ripol	2277.00		NIST Webbook
tb	610.05	K	Joback Method
tc	782.91	K	Joback Method
tf	305.72	K	Joback Method
vc	0.585	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.74	J/molxK	610.05	Joback Method
cpg	413.76	J/molxK	638.86	Joback Method
cpg	424.19	J/molxK	667.67	Joback Method

cpg	434.07	J/mol×K	696.48	Joback Method
cpg	443.45	J/mol×K	725.29	Joback Method
cpg	452.35	J/mol×K	754.10	Joback Method
cpg	460.83	J/mol×K	782.91	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=C75991616&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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