

(5E)-2,6-dimethyl-5,7-octadien-2,3-diol

Inchi:	InChI=1S/C10H18O2/c1-5-8(2)6-7-9(11)10(3,4)12/h5-6,9,11-12H,1,7H2,2-4H3/b8-6+
InchiKey:	BTHAWHOTHGQIKC-SOFGYWHQSA-N
Formula:	C10H18O2
SMILES:	C=CC(C)=CCC(O)C(C)(C)O
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
gf	-80.41	kJ/mol	Joback Method
hf	-335.36	kJ/mol	Joback Method
hfus	16.51	kJ/mol	Joback Method
hvap	68.90	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.641		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
tb	609.61	K	Joback Method
tc	785.25	K	Joback Method
tf	290.72	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.19	J/molxK	609.61	Joback Method
cpg	414.43	J/molxK	638.88	Joback Method
cpg	425.05	J/molxK	668.16	Joback Method
cpg	435.11	J/molxK	697.43	Joback Method
cpg	444.63	J/molxK	726.70	Joback Method
cpg	453.67	J/molxK	755.98	Joback Method
cpg	462.25	J/molxK	785.25	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=R334493&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
mccvol:	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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