

2,6-Dimethyl-3 (E),5 (Z),7-octatrien-2-ol

Other names:	2,6-Dimethyl-3(E),5(Z)-7-octatriene-2-ol
Inchi:	InChI=1S/C10H16O/c1-5-9(2)7-6-8-10(3,4)11/h5-8,11H,1H2,2-4H3/b8-6+,9-7-
InchiKey:	HYBLHNGOEIJQDA-FFELTBMSA-N
Formula:	C10H16O
SMILES:	C=CC(C)=CC=CC(C)(C)O
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
gf	139.07	kJ/mol	Joback Method
hf	-60.63	kJ/mol	Joback Method
hfus	16.14	kJ/mol	Joback Method
hvap	52.56	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.446		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
ripol	1815.00		NIST Webbook
ripol	1815.00		NIST Webbook
ripol	1815.00		NIST Webbook
tb	522.03	K	Joback Method
tc	709.57	K	Joback Method
tf	239.82	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.09	J/mol×K	522.03	Joback Method
cpg	341.99	J/mol×K	553.29	Joback Method
cpg	354.09	J/mol×K	584.54	Joback Method
cpg	365.44	J/mol×K	615.80	Joback Method
cpg	376.09	J/mol×K	647.06	Joback Method
cpg	386.11	J/mol×K	678.32	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R323329&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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