1,5,7-Octatrien-3-ol, 3,7-dimethyl-

Other names:	Hotrienol
	3,7-Dimethyl-1,5,7-octatrien-3-ol
	2,6-dimethyl-1,3,7-octatrien-6-ol
	3,7-dimethyl-1,5,7-octatriene-3-ol
	3,7-Dimethyl-octa-1,5,7-trien-3-ol
Inchi:	InChI=1S/C10H16O/c1-5-10(4,11)8-6-7-9(2)3/h5-7,11H,1-2,8H2,3-4H3/b7-6+
InchiKey:	ZJIQIJIQBTVTDY-VOTSOKGWSA-N
Formula:	C10H16O
SMILES:	C=CC(C)(O)CC=CC(=C)C
Mol. weight [g/mol]:	152.23
CAS:	29957-43-5

Physical Properties

Property code	Value	Unit	Source
gf	146.69	kJ/mol	Joback Method
hf	-52.42	kJ/mol	Joback Method
hfus	14.66	kJ/mol	Joback Method
hvap	51.94	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.446		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
rinpol	1115.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1106.00		NIST Webbook

rinpol	1108.00		NIST Webbook
rinpol	1107.70		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1108.00		NIST Webbook
ripol	1614.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1614.00		NIST Webbook
ripol	1621.00		NIST Webbook
ripol	1573.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1573.00		NIST Webbook
ripol	1605.00		NIST Webbook
ripol	1585.00		NIST Webbook
ripol	1605.00		NIST Webbook
ripol	1613.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1648.00		NIST Webbook
ripol	1613.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1605.00		NIST Webbook
ripol	1614.00		NIST Webbook
tb	514.55	K	Joback Method
tc	697.69	K	Joback Method
tf	243.14	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.52	J/mol×K	514.55	Joback Method
cpg	341.30	J/mol×K	545.07	Joback Method
cpg	353.32	J/mol×K	575.60	Joback Method
cpg	364.63	J/mol×K	606.12	Joback Method
cpg	375.27	J/mol×K	636.64	Joback Method
cpg	385.29	J/mol×K	667.16	Joback Method
cpg	394.75	J/mol×K	697.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29957435&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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