2-Cyclopenten-1-one, 4-hydroxy-3-methyl-2-(2-propenyl)-

Other names: 2-Cyclopenten-1-one, 2-allyl-4-hydroxy-3-methyl-
Allethrolon
Allethrolone
4-Hydroxy-3-methyl-2-(2-propenyl)-2-cyclopenten-1-one

Inchi: InChI=1S/C9H12O2/c1-3-4-7-6(2)8(10)5-9(7)11/h3,8,10H,1,4-5H2,2H3

InchiKey: KZYVOZABVXLALY-UHFFFAOYSA-N

Formula: C9H12O2

SMILES: C=CCC1=C(C)C(O)CC1=O

Mol. weight [g/mol]: 152.19

CAS: 551-45-1

Physical Properties

Property code	Value	Unit	Source
gf	-99.42	kJ/mol	Joback Method
hf	-298.27	kJ/mol	Joback Method
hfus	15.76	kJ/mol	Joback Method
hvap	57.76	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.213		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
tb	586.40	K	Joback Method
tc	789.42	K	Joback Method
tf	355.17	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.95	J/mol×K	586.40	Joback Method
cpg	322.03	J/mol×K	620.24	Joback Method
cpg	333.55	J/mol×K	654.07	Joback Method
cpg	344.49	J/mol×K	687.91	Joback Method
cpg	354.87	J/mol×K	721.75	Joback Method

cpg	364.68	J/mol×K	755.58	Joback Method
cpg	373.93	J/mol×K	789.42	Joback Method

Sources

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=C551451&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume