Acetophenone, 3'-allyl-4'-hydroxy-

Other names:	Ethanone, 1-(4-hydroxy-3-(2-propenyl)phenyl)-
	3'-Allyl-4'-hydroxyacetophenone
	3-Allyl-4-hydroxy-acetophenon
	3-Allyl-4-hydroxy-acetophenone
Inchi:	InChI=1S/C11H12O2/c1-3-4-10-7-9(8(2)12)5-6-11(10)13/h3,5-7,13H,1,4H2,2H3
InchiKey:	XVTCWUFLNLZPEJ-UHFFFAOYSA-N
Formula:	C11H12O2
SMILES:	C=CCc1cc(C(C)=O)ccc1O
Mol. weight [g/mol]:	176.21
CAS:	1132-05-4

Physical Properties

Property code	Value	Unit	Source
gf	-51.18	kJ/mol	Joback Method
hf	-209.77	kJ/mol	Joback Method
hfus	24.00	kJ/mol	Joback Method
hvap	62.11	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.323		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
tb	613.91	K	Joback Method
tc	841.77	K	Joback Method
tf	412.56	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.40	J/mol×K	613.91	Joback Method
cpg	364.55	J/mol×K	651.89	Joback Method
cpg	375.87	J/mol×K	689.86	Joback Method
cpg	386.45	J/mol×K	727.84	Joback Method
cpg	396.37	J/mol×K	765.82	Joback Method

cpg	405.71	J/mol×K	803.79	Joback Method
cpg	414.58	J/mol×K	841.77	Joback Method
dvisc	0.0008992	Pa×s	412.56	Joback Method
dvisc	0.0004319	Pa×s	446.12	Joback Method
dvisc	0.0002298	Pa×s	479.68	Joback Method
dvisc	0.0001328	Pa×s	513.24	Joback Method
dvisc	0.0000821	Pa×s	546.79	Joback Method
dvisc	0.0000537	Pa×s	580.35	Joback Method
dvisc	0.0000367	Pa×s	613.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1132054&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
dvisc:	Dynamic viscosity
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

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