3-Allyl-4-hydroxyacetophenone

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]: 176.22

Physical Properties

Property code	Value	Unit	Source
hfus	24.00	kJ/mol	Joback Method
logp	2.323		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
tb	559.53	K	Cheméo Relay (1.0)
tf	338.92	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.40	J/mol×K	613.91	Joback Method
cpg	414.58	J/mol×K	841.77	Joback Method
cpg	405.71	J/mol×K	803.79	Joback Method
cpg	396.37	J/mol×K	765.82	Joback Method
cpg	386.45	J/mol×K	727.84	Joback Method
cpg	375.87	J/mol×K	689.86	Joback Method
cpg	364.55	J/mol×K	651.89	Joback Method
dvisc	0.0001328	Pa×s	513.24	Joback Method
dvisc	0.0000367	Pa×s	613.91	Joback Method
dvisc	0.0000537	Pa×s	580.35	Joback Method
dvisc	0.0000821	Pa×s	546.79	Joback Method
dvisc	0.0008992	Pa×s	412.56	Joback Method
dvisc	0.0002298	Pa×s	479.68	Joback Method

dvisc	0.0004319	Pa×s	446.12	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1132054&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point