4-(1-Hydroxyallyl)-2-methoxyphenol

Inchi: InChI=1S/C10H12O3/c1-3-8(11)7-4-5-9(12)10(6-7)13-2/h3-6,8,11-12H,1H2,2H3
InchiKey: CAQJZUXHKMYJEF-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: C=CC(O)c1ccc(O)c(OC)c1
Mol. weight [g/mol]: 180.20
CAS: 112465-50-6

Physical Properties

Property code	Value	Unit	Source
gf	-174.94	kJ/mol	Joback Method
hf	-366.28	kJ/mol	Joback Method
hfus	21.56	kJ/mol	Joback Method
hvap	71.84	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.620		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
rinpol	1576.70		NIST Webbook
tb	651.32	K	Joback Method
tc	860.87	K	Joback Method
tf	419.41	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.84	J/mol×K	651.32	Joback Method
cpg	373.15	J/mol×K	686.24	Joback Method
cpg	382.86	J/mol×K	721.17	Joback Method
cpg	392.02	J/mol×K	756.09	Joback Method
cpg	400.69	J/mol×K	791.02	Joback Method
cpg	408.92	J/mol×K	825.94	Joback Method
cpg	416.77	J/mol×K	860.87	Joback Method
dvisc	0.0007556	Pa×s	419.41	Joback Method

dvisc	0.0002468	Pa×s	458.06	Joback Method
dvisc	0.0000960	Pa×s	496.71	Joback Method
dvisc	0.0000428	Pa×s	535.37	Joback Method
dvisc	0.0000212	Pa×s	574.02	Joback Method
dvisc	0.0000115	Pa×s	612.67	Joback Method
dvisc	0.0000067	Pa×s	651.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112465506&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume