1-Hydroxy-2-(prop-2-enyl)-4,5-methylenedioxyben

Inchi: InChI=1S/C10H10O3/c1-2-3-7-4-9-10(5-8(7)11)13-6-12-9/h2,4-5,11H,1,3,6H2
InchiKey: HSDKTWGTSNDEBZ-UHFFFAOYSA-N
Formula: C10H10O3
SMILES: C=CCc1cc2c(cc1O)OCO2
Mol. weight [g/mol]: 178.18
CAS: 19202-23-4

Physical Properties

Property code	Value	Unit	Source
gf	-44.09	kJ/mol	Joback Method
hf	-258.88	kJ/mol	Joback Method
hfus	32.44	kJ/mol	Joback Method
hvap	63.04	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	1.849		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
rinpol	1547.00		NIST Webbook
tb	607.45	K	Joback Method
tc	844.46	K	Joback Method
tf	439.20	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.75	J/mol×K	607.45	Joback Method
cpg	377.38	J/mol×K	804.96	Joback Method
cpg	368.87	J/mol×K	765.46	Joback Method
cpg	359.88	J/mol×K	725.95	Joback Method
cpg	350.28	J/mol×K	686.45	Joback Method
cpg	339.95	J/mol×K	646.95	Joback Method
cpg	385.54	J/mol×K	844.46	Joback Method
dvisc	0.0000755	Pa×s	607.45	Joback Method

dvisc	0.0001024	Pa×s	579.41	Joback Method
dvisc	0.0001431	Pa×s	551.37	Joback Method
dvisc	0.0002074	Pa×s	523.33	Joback Method
dvisc	0.0003134	Pa×s	495.28	Joback Method
dvisc	0.0004976	Pa×s	467.24	Joback Method
dvisc	0.0008382	Pa×s	439.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19202234&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