Hydroxy chavicol

Inchi: InChI=1S/C9H10O2/c1-2-3-7-4-5-8(10)9(11)6-7/h2,4-6,10-11H,1,3H2
InchiKey: FHEHIXJLCWUPCZ-UHFFFAOYSA-N
Formula: C9H10O2
SMILES: C=CCc1ccc(O)c(O)c1
Mol. weight [g/mol]: 150.17
CAS: 1126-61-0

Physical Properties

Property code	Value	Unit	Source
gf	-84.09	kJ/mol	Joback Method
hf	-221.75	kJ/mol	Joback Method
hfus	23.39	kJ/mol	Joback Method
hvap	63.26	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.826		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	5022.80	kPa	Joback Method
rinpol	1522.00		NIST Webbook
rinpol	1522.00		NIST Webbook
tb	589.92	K	Joback Method
tc	828.66	K	Joback Method
tf	439.29	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.44	J/mol×K	589.92	Joback Method
cpg	304.85	J/mol×K	629.71	Joback Method
cpg	314.42	J/mol×K	669.50	Joback Method
cpg	323.29	J/mol×K	709.29	Joback Method
cpg	331.62	J/mol×K	749.08	Joback Method
cpg	339.56	J/mol×K	788.87	Joback Method
cpg	347.27	J/mol×K	828.66	Joback Method

dvisc	0.0002846	Pa×s	439.29	Joback Method
dvisc	0.0001335	Pa×s	464.39	Joback Method
dvisc	0.0000677	Pa×s	489.50	Joback Method
dvisc	0.0000367	Pa×s	514.61	Joback Method
dvisc	0.0000210	Pa×s	539.71	Joback Method
dvisc	0.0000127	Pa×s	564.81	Joback Method
dvisc	0.0000080	Pa×s	589.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1126610&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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