4-(1 E)-3-hydroxy-1-propenyl-2-methoxyphenol

Other names: 3-(4-Hydroxy-3-methoxyphenyl)-2-propenyl alcohol (cis-coniferyl alcohol)
2-Propen-1-ol, 3-(4-hydroxy-3-methoxyphenyl), (E)-
Inchi: InChI=1S/C10H12O3/c1-13-10-7-8(3-2-6-11)4-5-9(10)12/h2-5,7,11-12H,6H2,1H3/b3-2+
InchiKey: JMFRWRFFLBVWSI-NSCUHMNNSA-N
Formula: C10H12O3
SMILES: COc1cc(C=CCO)ccc1O
Mol. weight [g/mol]: 180.20
CAS: 69056-21-9

Physical Properties

Property code	Value	Unit	Source
gf	-180.12	kJ/mol	Joback Method
hf	-369.21	kJ/mol	Joback Method
hfus	26.57	kJ/mol	Joback Method
hvap	72.85	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.406		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
rinpol	1727.00		NIST Webbook
rinpol	1683.00		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1683.00		NIST Webbook
ripol	2832.00		NIST Webbook
tb	659.24	K	Joback Method
tc	869.04	K	Joback Method
tf	431.09	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.86	J/mol×K	659.24	Joback Method
cpg	371.97	J/mol×K	694.21	Joback Method

cpg	381.51	J/mol×K	729.17	Joback Method
cpg	390.53	J/mol×K	764.14	Joback Method
cpg	399.09	J/mol×K	799.11	Joback Method
cpg	407.27	J/mol×K	834.08	Joback Method
cpg	415.12	J/mol×K	869.04	Joback Method
dvisc	0.0004866	Pa×s	431.09	Joback Method
dvisc	0.0001709	Pa×s	469.12	Joback Method
dvisc	0.0000702	Pa×s	507.14	Joback Method
dvisc	0.0000327	Pa×s	545.16	Joback Method
dvisc	0.0000168	Pa×s	583.19	Joback Method
dvisc	0.0000094	Pa×s	621.22	Joback Method
dvisc	0.0000056	Pa×s	659.24	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C69056219&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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume