4-((1E)-Hydroxy-1-propenyl]-2-methoxyphenol

Inchi: InChI=1S/C10H12O3/c1-3-8(11)7-4-5-9(12)10(6-7)13-2/h3-6,11-12H,1-2H3/b8-3+
InchiKey: BOVBOPAVCSURFY-FPYGCLRLSA-N
Formula: C10H12O3
SMILES: CC=C(O)c1ccc(O)c(OC)c1
Mol. weight [g/mol]: 180.20

Physical Properties

Property code	Value	Unit	Source
gf	-188.67	kJ/mol	Joback Method
hf	-379.00	kJ/mol	Joback Method
hfus	25.26	kJ/mol	Joback Method
hvap	72.93	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	2.320		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
rinpol	1609.00		NIST Webbook
tb	659.12	K	Joback Method
tc	872.26	K	Joback Method
tf	417.13	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.60	J/mol×K	659.12	Joback Method
cpg	371.84	J/mol×K	694.64	Joback Method
cpg	381.49	J/mol×K	730.17	Joback Method
cpg	390.62	J/mol×K	765.69	Joback Method
cpg	399.29	J/mol×K	801.21	Joback Method
cpg	407.56	J/mol×K	836.73	Joback Method
cpg	415.51	J/mol×K	872.26	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R613291&Units=SI

Legend

cpg:	Ideal gas heat capacity
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