4-(1-Propenyl)-2,6-dimethoxyphenol (trans-propenylsyringol)

Other names: trans-propenylsyringol
Inchi: InChI=1S/C11H14O3/c1-4-8-14-11-9(12-2)6-5-7-10(11)13-3/h4-8H,1-3H3/b8-4+
InchiKey: VCUJKQLQRUJWCJ-XBXARRHUSA-N
Formula: C11H14O3
SMILES: CC=COc1c(OC)cccc1OC
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
gf	-99.89	kJ/mol	Joback Method
hf	-336.22	kJ/mol	Joback Method
hfus	21.28	kJ/mol	Joback Method
hvap	50.87	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.616		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1708.50		NIST Webbook
tb	559.14	K	Joback Method
tc	767.11	K	Joback Method
tf	326.80	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.53	J/mol×K	559.14	Joback Method
cpg	371.51	J/mol×K	593.80	Joback Method
cpg	384.86	J/mol×K	628.46	Joback Method
cpg	397.58	J/mol×K	663.12	Joback Method
cpg	409.66	J/mol×K	697.78	Joback Method
cpg	421.10	J/mol×K	732.45	Joback Method
cpg	431.88	J/mol×K	767.11	Joback Method
dvisc	0.0007880	Pa×s	326.80	Joback Method

dvisc	0.0004661	Pa×s	365.52	Joback Method
dvisc	0.0003049	Pa×s	404.25	Joback Method
dvisc	0.0002148	Pa×s	442.97	Joback Method
dvisc	0.0001601	Pa×s	481.69	Joback Method
dvisc	0.0001247	Pa×s	520.42	Joback Method
dvisc	0.0001005	Pa×s	559.14	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=R205182&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