3-(4-Hydroxy-3,5-dimethoxyphenyl)-2-propen-1-al (sinapaldehyde)

Other names: trans-Sinapaldehyde
Inchi: InChI=1S/C11H12O4/c1-14-9-6-8(4-3-5-12)7-10(15-2)11(9)13/h3-7,13H,1-2H3/b4-3+
InchiKey: CDICDSOGTRCHMG-ONEGZZNKSA-N
Formula: C11H12O4
SMILES: COc1cc(C=CC=O)cc(OC)c1O
Mol. weight [g/mol]: 208.21
CAS: 4206-58-0

Physical Properties

Property code	Value	Unit	Source
gf	-249.03	kJ/mol	Joback Method
hf	-466.89	kJ/mol	Joback Method
hfus	28.16	kJ/mol	Joback Method
hvap	68.19	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.621		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	2011.10		NIST Webbook
rinpol	2011.10		NIST Webbook
tb	666.00	K	Joback Method
tc	888.57	K	Joback Method
tf	458.29	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.69	J/mol×K	666.00	Joback Method
cpg	449.53	J/mol×K	851.48	Joback Method
cpg	440.47	J/mol×K	814.38	Joback Method
cpg	430.90	J/mol×K	777.29	Joback Method
cpg	420.78	J/mol×K	740.19	Joback Method
cpg	410.06	J/mol×K	703.10	Joback Method

cpg	458.15	J/mol×K	888.57	Joback Method
dvisc	0.0000162	Pa×s	666.00	Joback Method
dvisc	0.0000229	Pa×s	631.38	Joback Method
dvisc	0.0000337	Pa×s	596.76	Joback Method
dvisc	0.0000520	Pa×s	562.14	Joback Method
dvisc	0.0000850	Pa×s	527.53	Joback Method
dvisc	0.0001487	Pa×s	492.91	Joback Method
dvisc	0.0002831	Pa×s	458.29	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4206580&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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