Coniferyl aldehyde

Other names:	2-Propenal, 3-(4-hydroxy-3-methoxyphenyl)-
	3-Methoxy-4-hydroxycinnamaldehyde
	4-Hydroxy-3-methoxycinnamaldehyde
	Coniferaldehyde
	Coniferylic aldehyde
	Cinnamaldehyde, 4-hydroxy-3-methoxy-
	CONIFERYL ALDEHYDE-1
	2-Propenal, 3-(4-hydroxy-3-methoxyphenyl), (E)-
	3-methoxy-4-hydroxycinnamaldehyde (coniferilic aldehyde)
	4'-hydroxy-3'-methoxycinnamaldehyde
Inchi:	InChI=1S/C10H10O3/c1-13-10-7-8(3-2-6-11)4-5-9(10)12/h2-7,12H,1H3/b3-2+
InchiKey:	DKZBBWMURDFHNE-NSCUHMNNSA-N
Formula:	C10H10O3
SMILES:	COc1cc(C=CC=O)ccc1O
Mol. weight [g/mol]:	178.18
CAS:	458-36-6

Physical Properties

Property code	Value	Unit	Source
gf	-142.82	kJ/mol	Joback Method
hf	-302.56	kJ/mol	Joback Method
hfus	24.77	kJ/mol	Joback Method
hvap	62.89	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.613		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
rinpol	1676.00		NIST Webbook
rinpol	1751.80		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1741.00		NIST Webbook
rinpol	1741.00		NIST Webbook
ripol	3038.00		NIST Webbook
tb	615.72	K	Joback Method
tc	844.66	K	Joback Method
tf	412.27	K	Joback Method

vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.26	J/mol×K	615.72	Joback Method
cpg	377.06	J/mol×K	806.51	Joback Method
cpg	368.65	J/mol×K	768.35	Joback Method
cpg	359.75	J/mol×K	730.19	Joback Method
cpg	350.26	J/mol×K	692.03	Joback Method
cpg	340.13	J/mol×K	653.88	Joback Method
cpg	385.04	J/mol×K	844.66	Joback Method
dvisc	0.0000290	Pa×s	615.72	Joback Method
dvisc	0.0000425	Pa×s	581.81	Joback Method
dvisc	0.0000654	Pa×s	547.90	Joback Method
dvisc	0.0001063	Pa×s	514.00	Joback Method
dvisc	0.0001852	Pa×s	480.09	Joback Method
dvisc	0.0003509	Pa×s	446.18	Joback Method
dvisc	0.0007386	Pa×s	412.27	Joback Method

Sources

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=C458366&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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