4-Hydroxy-2-methoxycinnamaldehyde

Other names:	(2 E)-3-(4-hydroxy-2-methoxyphenyl)-2-propenal
Inchi:	InChI=1S/C10H10O3/c1-13-10-7-9(12)5-4-8(10)3-2-6-11/h2-7,12H,1H3/b3-2+
InchiKey:	MRCGVXARHKOYKU-NSCUHMNNSA-N
Formula:	C10H10O3
SMILES:	COc1cc(O)ccc1C=CC=O
Mol. weight [g/mol]:	178.18
CAS:	127321-19-1

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	1740.00		NIST Webbook
ripol	2681.00		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	340.13	J/mol×K	653.88	Joback Method
cpg	350.26	J/mol×K	692.03	Joback Method
cpg	359.75	J/mol×K	730.19	Joback Method
cpg	368.65	J/mol×K	768.35	Joback Method
cpg	377.06	J/mol×K	806.51	Joback Method

cpg	385.04	J/mol×K	844.66	Joback Method
dvisc	0.0007386	Pa×s	412.27	Joback Method
dvisc	0.0003509	Pa×s	446.18	Joback Method
dvisc	0.0001852	Pa×s	480.09	Joback Method
dvisc	0.0001063	Pa×s	514.00	Joback Method
dvisc	0.0000654	Pa×s	547.90	Joback Method
dvisc	0.0000425	Pa×s	581.81	Joback Method
dvisc	0.0000290	Pa×s	615.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C127321191&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

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