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