2-Propenoic acid, 3-(2-hydroxyphenyl)-, methyl ester

Other names: Methyl o-coumarate
Cinnamic acid, O-hydroxy-, methyl ester
Methyl o-hydroxycinnamate
Methyl ester of O-hydroxycinnamic acid
Methyl 3-(2-hydroxyphenyl)-2-propenoate
O-Hydroxycinnamic acid, methyl ester

Inchi: InChI=1S/C10H10O3/c1-13-10(12)7-6-8-4-2-3-5-9(8)11/h2-7,11H,1H3/b7-6+

InchiKey: YMXREWKKROWOSO-VOTSOKGWSA-N

Formula: C10H10O3

SMILES: COC(=O)C=Cc1ccccc1O

Mol. weight [g/mol]: 178.18

CAS: 20883-98-1

Physical Properties

Property code	Value	Unit	Source
gf	-162.59	kJ/mol	Joback Method
hf	-318.09	kJ/mol	Joback Method
hfus	24.47	kJ/mol	Joback Method
hvap	62.26	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.578		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
rinpol	1430.00		NIST Webbook
rinpol	1430.00		NIST Webbook
tb	615.95	K	Joback Method
tc	849.16	K	Joback Method
tf	407.68	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.29	J/mol×K	615.95	Joback Method

cpg	378.94	J/mol×K	810.29	Joback Method
cpg	370.29	J/mol×K	771.43	Joback Method
cpg	361.09	J/mol×K	732.56	Joback Method
cpg	351.25	J/mol×K	693.69	Joback Method
cpg	340.68	J/mol×K	654.82	Joback Method
cpg	387.11	J/mol×K	849.16	Joback Method
dvisc	0.0000267	Pa×s	615.95	Joback Method
dvisc	0.0000399	Pa×s	581.24	Joback Method
dvisc	0.0000628	Pa×s	546.53	Joback Method
dvisc	0.0001050	Pa×s	511.82	Joback Method
dvisc	0.0001891	Pa×s	477.10	Joback Method
dvisc	0.0003738	Pa×s	442.39	Joback Method
dvisc	0.0008298	Pa×s	407.68	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20883981&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