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

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

Inchi: InChI=1S/C10H10O3/c1-13-10(12)6-5-8-3-2-4-9(11)7-8/h2-7,11H,1H3/b6-5+

InchiKey: PKALKWFZXXGNJD-AATRIKPKSA-N

Formula: C10H10O3

SMILES: COC(=O)C=Cc1cccc(O)c1

Mol. weight [g/mol]: 178.18

CAS: 3943-95-1

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	1690.00		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	340.68	J/mol×K	654.82	Joback Method
cpg	351.25	J/mol×K	693.69	Joback Method

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

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C3943951&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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