3,4-Methylenedioxycinnamic acid

Other names:	2-Propenoic acid, 3-(1,3-benzodioxol-5-yl)-
	3,4-Methylenedioxybenzene-3-acrylic acid
	3-(1,3-Benzodioxol-5-yl)-2-propenoic acid
	3-(3,4-Methylenedioxyphenyl)propenoic acid
	Acetic acid, piperonylidene-
	Cinnamic acid, 3,4-(methylenebis(oxy))-
	Cinnamic acid, 3,4-(methylenedioxy)-
	trans-3,4-(methylenedioxy)cinnamic acid
Inchi:	InChI=1S/C10H8O4/c11-10(12)4-2-7-1-3-8-9(5-7)14-6-13-8/h1-5H,6H2,(H,11,12)/b4-2+
InchiKey:	QFQYZMGOKIROEC-DUXPYHPUSA-N
Formula:	C10H8O4
SMILES:	O=C(O)C=Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	192.17
CAS:	2373-80-0

Physical Properties

Property code	Value	Unit	Source
chs	-4471.90	kJ/mol	NIST Webbook
chs	-4472.30	kJ/mol	NIST Webbook
gf	-162.83	kJ/mol	Joback Method
hf	-354.59	kJ/mol	Joback Method
hfs	-605.80	kJ/mol	NIST Webbook
hfus	33.83	kJ/mol	Joback Method
hvap	74.08	kJ/mol	Joback Method
log10ws	-3.19		Aqueous Solubility Prediction Method
logp	1.513		Crippen Method
mcvol	132.020	ml/mol	McGowan Method
pc	4299.92	kPa	Joback Method
tb	680.36	K	Joback Method
tc	900.48	K	Joback Method
tf	434.91	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.06	J/mol×K	680.36	Joback Method
cpg	377.16	J/mol×K	863.80	Joback Method
cpg	370.35	J/mol×K	827.11	Joback Method
cpg	363.11	J/mol×K	790.42	Joback Method
cpg	355.36	J/mol×K	753.73	Joback Method
cpg	347.03	J/mol×K	717.05	Joback Method
cpg	383.61	J/mol×K	900.48	Joback Method
dvisc	0.0001182	Pa×s	680.36	Joback Method
dvisc	0.0001614	Pa×s	639.45	Joback Method
dvisc	0.0002300	Pa×s	598.54	Joback Method
dvisc	0.0003450	Pa×s	557.63	Joback Method
dvisc	0.0005521	Pa×s	516.73	Joback Method
dvisc	0.0009577	Pa×s	475.82	Joback Method
dvisc	0.0018426	Pa×s	434.91	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2373800&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume