3-Methylcinnamic acid

Other names: 2-Propenoic acid, 3-(3-methylphenyl)-
Cinnamic acid, m-methyl-
m-Methylcinnamic acid
Inchi: InChI=1S/C10H10O2/c1-8-3-2-4-9(7-8)5-6-10(11)12/h2-7H,1H3,(H,11,12)/b6-5+
InchiKey: JZINNAKNHHQBOS-AATRIKPKSA-N
Formula: C10H10O2
SMILES: Cc1cccc(C=CC(=O)O)c1
Mol. weight [g/mol]: 162.19
CAS: 3029-79-6

Physical Properties

Property code	Value	Unit	Source
gf	-49.42	kJ/mol	Joback Method
hf	-172.26	kJ/mol	Joback Method
hfus	21.20	kJ/mol	Joback Method
hvap	64.18	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.093		Crippen Method
mcvol	131.140	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	610.07	K	Joback Method
tc	819.56	K	Joback Method
tf	347.07	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.72	J/mol×K	610.07	Joback Method
cpg	316.15	J/mol×K	644.98	Joback Method
cpg	325.90	J/mol×K	679.90	Joback Method
cpg	335.02	J/mol×K	714.81	Joback Method
cpg	343.54	J/mol×K	749.73	Joback Method
cpg	351.51	J/mol×K	784.64	Joback Method

cpg	358.96	J/mol×K	819.56	Joback Method
dvisc	0.0038653	Pa×s	347.07	Joback Method
dvisc	0.0013852	Pa×s	390.90	Joback Method
dvisc	0.0006105	Pa×s	434.74	Joback Method
dvisc	0.0003127	Pa×s	478.57	Joback Method
dvisc	0.0001792	Pa×s	522.40	Joback Method
dvisc	0.0001119	Pa×s	566.24	Joback Method
dvisc	0.0000748	Pa×s	610.07	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3029796&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume