p-Chlorocinnamic acid

Other names:	4-Chlorocinnamic acid
	trans-4-Chlorocinnamic acid
	2-Propenoic acid, 3-(4-chlorophenyl)-
	Cinnamic acid, p-chloro-
	3-(p-Chlorophenyl)acrylic acid
Inchi:	InChI=1S/C9H7ClO2/c10-8-4-1-7(2-5-8)3-6-9(11)12/h1-6H,(H,11,12)/b6-3+
InchiKey:	GXLIFJYFGMHYDY-ZZXKWVIFSA-N
Formula:	C9H7ClO2
SMILES:	O=C(O)C=Cc1ccc(Cl)cc1
Mol. weight [g/mol]:	182.60
CAS:	1615-02-7

Physical Properties

Property code	Value	Unit	Source
gf	-69.77	kJ/mol	Joback Method
hf	-167.36	kJ/mol	Joback Method
hfus	22.80	kJ/mol	Joback Method
hvap	66.33	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.438		Crippen Method
mcvol	129.290	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
tb	624.62	K	Joback Method
tc	841.31	K	Joback Method
tf	365.72	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.40	J/mol×K	624.62	Joback Method
cpg	290.14	J/mol×K	660.73	Joback Method
cpg	298.25	J/mol×K	696.85	Joback Method
cpg	305.78	J/mol×K	732.96	Joback Method

cpg	312.76	J/mol×K	769.08	Joback Method
cpg	319.25	J/mol×K	805.19	Joback Method
cpg	325.27	J/mol×K	841.31	Joback Method
dvisc	0.0030646	Pa×s	365.72	Joback Method
dvisc	0.0011985	Pa×s	408.87	Joback Method
dvisc	0.0005607	Pa×s	452.02	Joback Method
dvisc	0.0002995	Pa×s	495.17	Joback Method
dvisc	0.0001769	Pa×s	538.32	Joback Method
dvisc	0.0001129	Pa×s	581.47	Joback Method
dvisc	0.0000767	Pa×s	624.62	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1615027&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