

2-Chlorocinnamic acid

Other names:	o-Chlorocinnamic acid 2-Propenoic acid, 3-(2-chlorophenyl)- Cinnamic acid, o-chloro-
Inchi:	InChI=1S/C9H7ClO2/c10-8-4-2-1-3-7(8)5-6-9(11)12/h1-6H,(H,11,12)/b6-5+
InchiKey:	KJRRTHHNKJBVBO-AATRIKPKSA-N
Formula:	C9H7ClO2
SMILES:	O=C(O)C=Cc1ccccc1Cl
Mol. weight [g/mol]:	182.60
CAS:	3752-25-8

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/molxK	624.62	Joback Method
cpg	319.25	J/molxK	805.19	Joback Method
cpg	312.76	J/molxK	769.08	Joback Method
cpg	305.78	J/molxK	732.96	Joback Method
cpg	298.25	J/molxK	696.85	Joback Method
cpg	290.14	J/molxK	660.73	Joback Method

cpg	325.27	J/mol×K	841.31	Joback Method
dvisc	0.0000767	Paxs	624.62	Joback Method
dvisc	0.0001129	Paxs	581.47	Joback Method
dvisc	0.0001769	Paxs	538.32	Joback Method
dvisc	0.0002995	Paxs	495.17	Joback Method
dvisc	0.0005607	Paxs	452.02	Joback Method
dvisc	0.0011985	Paxs	408.87	Joback Method
dvisc	0.0030646	Paxs	365.72	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=C3752258&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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