

2,6-Dichlorocinnamic acid

Other names:	2-Propenoic acid, 3-(2,6-dichlorophenyl)-
Inchi:	InChI=1S/C9H6Cl2O2/c10-7-2-1-3-8(11)6(7)4-5-9(12)13/h1-5H,(H,12,13)/b5-4+
InchiKey:	OIPVGRCXMFBNAN-SNAWJCMRSA-N
Formula:	C9H6Cl2O2
SMILES:	O=C(O)C=Cc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	217.05
CAS:	5345-89-1

Physical Properties

Property code	Value	Unit	Source
gf	-91.33	kJ/mol	Joback Method
hf	-194.57	kJ/mol	Joback Method
hfus	26.61	kJ/mol	Joback Method
hvap	71.38	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	3.091		Crippen Method
mcvol	141.530	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	667.03	K	Joback Method
tc	887.93	K	Joback Method
tf	408.16	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.67	J/mol×K	667.03	Joback Method
cpg	307.42	J/mol×K	703.85	Joback Method
cpg	314.60	J/mol×K	740.66	Joback Method
cpg	321.25	J/mol×K	777.48	Joback Method
cpg	327.43	J/mol×K	814.30	Joback Method
cpg	333.16	J/mol×K	851.11	Joback Method
cpg	338.49	J/mol×K	887.93	Joback Method
dvisc	0.0015871	Pa×s	408.16	Joback Method

dvisc	0.0007202	Pa×s	451.31	Joback Method
dvisc	0.0003751	Pa×s	494.45	Joback Method
dvisc	0.0002170	Pa×s	537.60	Joback Method
dvisc	0.0001361	Pa×s	580.74	Joback Method
dvisc	0.0000911	Pa×s	623.88	Joback Method
dvisc	0.0000642	Pa×s	667.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5345891&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

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