

trans-«beta»-Chloroacrylic acid

Other names:	trans-3-Chloroacrylic acid 2-Propenoic acid, 3-chloro-, (E)- (E)-3-Chloroacrylic acid Acrylic acid, 3-chloro-, (E)- Acrylic acid, 3-chloro-, trans-
Inchi:	InChI=1S/C3H3ClO2/c4-2-1-3(5)6/h1-2H,(H,5,6)/b2-1+
InchiKey:	MHMUCYJKZUZMNJ-OWOJBTEDSA-N
Formula:	C3H3ClO2
SMILES:	O=C(O)C=CCl
Mol. weight [g/mol]:	106.51
CAS:	2345-61-1

Physical Properties

Property code	Value	Unit	Source
gf	-223.07	kJ/mol	Joback Method
hf	-268.58	kJ/mol	Joback Method
hfus	13.61	kJ/mol	Joback Method
hvap	50.04	kJ/mol	Joback Method
log10ws	-0.68		Crippen Method
logp	0.823		Crippen Method
mcvol	68.510	ml/mol	McGowan Method
pc	5602.57	kPa	Joback Method
tb	455.68	K	Joback Method
tc	646.19	K	Joback Method
tf	259.16	K	Joback Method
vc	0.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	112.78	J/mol×K	455.68	Joback Method
cpg	117.08	J/mol×K	487.43	Joback Method
cpg	121.10	J/mol×K	519.18	Joback Method
cpg	124.87	J/mol×K	550.93	Joback Method

cpg	128.39	J/mol×K	582.68	Joback Method
cpg	131.68	J/mol×K	614.44	Joback Method
cpg	134.76	J/mol×K	646.19	Joback Method
dvisc	0.0224526	Pa×s	259.16	Joback Method
dvisc	0.0069569	Pa×s	291.91	Joback Method
dvisc	0.0027305	Pa×s	324.67	Joback Method
dvisc	0.0012720	Pa×s	357.42	Joback Method
dvisc	0.0006737	Pa×s	390.17	Joback Method
dvisc	0.0003937	Pa×s	422.93	Joback Method
dvisc	0.0002486	Pa×s	455.68	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C2345611&Units=SI

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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