

Alpha-chloroacrylic acid

Other names:	2-Chloroacrylic acid 2-Propenoic acid, 2-chloro- Acrylic acid, 2-chloro- Alpha-chloroacrylic acid
Inchi:	InChI=1S/C3H3ClO2/c1-2(4)3(5)6/h1H2,(H,5,6)
InchiKey:	SZTBMHYHIYNGYIA-UHFFFAOYSA-N
Formula:	C3H3ClO2
SMILES:	C=C(Cl)C(=O)O
Mol. weight [g/mol]:	106.51

Physical Properties

Property code	Value	Unit	Source
af	0.5821		Cheméo Relay (1.0)
gf	-224.00	kJ/mol	Joback Method
hf	-348.73	kJ/mol	Cheméo Relay (1.0)
hfus	10.82	kJ/mol	Joback Method
hvap	49.07	kJ/mol	Cheméo Relay (1.0)
ie	10.23	eV	Cheméo Relay (1.0)
log10ws	-0.29		Cheméo Relay (1.0)
logp	0.823		Crippen Method
mcvol	68.510	ml/mol	McGowan Method
pc	5560.87	kPa	Joback Method
tb	436.42	K	Cheméo Relay (1.0)
tc	651.47	K	Cheméo Relay (1.0)
tf	352.52	K	Cheméo Relay (1.0)
vc	0.244	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.47	J/mol×K	448.08	Joback Method
cpg	118.68	J/mol×K	479.58	Joback Method
cpg	122.65	J/mol×K	511.09	Joback Method
cpg	126.39	J/mol×K	542.59	Joback Method

cpg	129.91	J/mol×K	574.10	Joback Method
cpg	133.23	J/mol×K	605.60	Joback Method
cpg	136.35	J/mol×K	637.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C598798&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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