

Chloroethiolacetic acid

Other names:	«alpha»-Chloroethioacetic acid
Inchi:	InChI=1S/C2H3ClOS/c3-1-2(4)5/h1H2,(H,4,5)
InchiKey:	IRYMZPFJICXSLB-UHFFFAOYSA-N
Formula:	C2H3ClOS
SMILES:	O=C(S)CCI
Mol. weight [g/mol]:	110.56
CAS:	867-49-2

Physical Properties

Property code	Value	Unit	Source
gf	-145.50	kJ/mol	Joback Method
hf	-174.45	kJ/mol	Joback Method
hfus	10.77	kJ/mol	Joback Method
hvap	37.91	kJ/mol	Joback Method
log10ws	-0.66		Crippen Method
logp	0.682		Crippen Method
mcvol	69.200	ml/mol	McGowan Method
pc	5739.21	kPa	Joback Method
tb	399.32	K	Joback Method
tc	617.13	K	Joback Method
tf	228.61	K	Joback Method
vc	0.257	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	99.79	J/mol×K	399.32	Joback Method
cpg	104.09	J/mol×K	435.62	Joback Method
cpg	108.16	J/mol×K	471.92	Joback Method
cpg	112.01	J/mol×K	508.22	Joback Method
cpg	115.64	J/mol×K	544.53	Joback Method
cpg	119.07	J/mol×K	580.83	Joback Method
cpg	122.29	J/mol×K	617.13	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C867492&Units=SI

Legend

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
h vap:	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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