(S)-(-)-2-Chloropropionic acid

Other names: Propanoic acid, 2-chloro-, (2S)-
(S) 2-chloropropionic acid
Inchi: InChI=1S/C3H5ClO2/c1-2(4)3(5)6/h2H,1H3,(H,5,6)/t2-/m1/s1
InchiKey: GAWAYYRQGQZKCR-UWTATZPHSA-N
Formula: C3H5ClO2
SMILES: CC(Cl)C(=O)O
Mol. weight [g/mol]: 108.52
CAS: 29617-66-1

Physical Properties

Property code	Value	Unit	Source
gf	-305.73	kJ/mol	Joback Method
hf	-391.08	kJ/mol	Joback Method
hfus	9.89	kJ/mol	Joback Method
hvap	64.90 ± 0.50	kJ/mol	NIST Webbook
log10ws	-0.44		Crippen Method
logp	0.698		Crippen Method
mcvol	72.810	ml/mol	McGowan Method
pc	5251.00	kPa	Joback Method
tb	451.08	K	Joback Method
tc	636.85	K	Joback Method
tf	249.24	K	Joback Method
vc	0.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.29	J/mol×K	451.08	Joback Method
cpg	135.44	J/mol×K	482.04	Joback Method
cpg	140.36	J/mol×K	513.00	Joback Method
cpg	145.04	J/mol×K	543.96	Joback Method
cpg	149.49	J/mol×K	574.92	Joback Method
cpg	153.72	J/mol×K	605.89	Joback Method
cpg	157.73	J/mol×K	636.85	Joback Method

dvisc	0.0423025	Pa×s	249.24	Joback Method
dvisc	0.0112935	Pa×s	282.88	Joback Method
dvisc	0.0039921	Pa×s	316.52	Joback Method
dvisc	0.0017233	Pa×s	350.16	Joback Method
dvisc	0.0008619	Pa×s	383.80	Joback Method
dvisc	0.0004820	Pa×s	417.44	Joback Method
dvisc	0.0002940	Pa×s	451.08	Joback Method
hvapt	63.40	kJ/mol	307.50	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29617661&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
hvapt: Enthalpy of vaporization at a given temperature
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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