

Alpha-bromo alpha-chloro-propionic acid

Inchi:	InChI=1S/C3H4BrClO2/c1-3(4,5)2(6)7/h1H3,(H,6,7)
InchiKey:	DQCULHMEDFODNL-UHFFFAOYSA-N
Formula:	C3H4BrClO2
SMILES:	CC(Cl)(Br)C(=O)O
Mol. weight [g/mol]:	187.42
CAS:	92018-32-1

Physical Properties

Property code	Value	Unit	Source
gf	-286.13	kJ/mol	Joback Method
hf	-368.22	kJ/mol	Joback Method
hfus	11.28	kJ/mol	Joback Method
hvap	55.22	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.421		Crippen Method
mcvol	90.310	ml/mol	McGowan Method
pc	5917.16	kPa	Joback Method
tb	514.45	K	Joback Method
tc	723.90	K	Joback Method
tf	326.46	K	Joback Method
vc	0.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.30	J/molxK	514.45	Joback Method
cpg	163.31	J/molxK	549.36	Joback Method
cpg	167.88	J/molxK	584.27	Joback Method
cpg	172.03	J/molxK	619.18	Joback Method
cpg	175.80	J/molxK	654.09	Joback Method
cpg	179.24	J/molxK	688.99	Joback Method
cpg	182.37	J/molxK	723.90	Joback Method
dvisc	0.0093909	Paxs	326.46	Joback Method
dvisc	0.0039217	Paxs	357.79	Joback Method

dvisc	0.0018850	Paxs	389.12	Joback Method
dvisc	0.0010106	Paxs	420.46	Joback Method
dvisc	0.0005907	Paxs	451.79	Joback Method
dvisc	0.0003702	Paxs	483.12	Joback Method
dvisc	0.0002456	Paxs	514.45	Joback Method

Sources

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=C92018321&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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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