

2-Bromopropionyl chloride

Other names:	«alpha»-Bromopropionyl chloride Propanoyl chloride, 2-bromo-
Inchi:	InChI=1S/C3H4BrClO/c1-2(4)3(5)6/h2H,1H3
InchiKey:	OZGMODDEIHYPY-UHFFFAOYSA-N
Formula:	C3H4BrClO
SMILES:	CC(Br)C(=O)Cl
Mol. weight [g/mol]:	171.42
CAS:	7148-74-5

Physical Properties

Property code	Value	Unit	Source
gf	-154.59	kJ/mol	Joback Method
hf	-212.52	kJ/mol	Joback Method
hfus	11.08	kJ/mol	Joback Method
hvap	39.45	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	1.535		Crippen Method
mvol	84.440	ml/mol	McGowan Method
pc	5080.25	kPa	Joback Method
tb	425.06	K	Joback Method
tc	639.62	K	Joback Method
tf	248.22	K	Joback Method
vc	0.315	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.91	J/mol×K	425.06	Joback Method
cpg	130.44	J/mol×K	460.82	Joback Method
cpg	135.63	J/mol×K	496.58	Joback Method
cpg	140.49	J/mol×K	532.34	Joback Method
cpg	145.04	J/mol×K	568.10	Joback Method
cpg	149.29	J/mol×K	603.86	Joback Method
cpg	153.25	J/mol×K	639.62	Joback Method

dvisc	0.0044204	Paxs	248.22	Joback Method
dvisc	0.0024999	Paxs	277.69	Joback Method
dvisc	0.0015772	Paxs	307.17	Joback Method
dvisc	0.0010786	Paxs	336.64	Joback Method
dvisc	0.0007842	Paxs	366.11	Joback Method
dvisc	0.0005979	Paxs	395.59	Joback Method
dvisc	0.0004733	Paxs	425.06	Joback Method

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=C7148745&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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