Bromoacetyl chloride

Other names: Acetyl chloride, bromo-
Inchi: InChI=1S/C2H2BrClO/c3-1-2(4)5/h1H2
InchiKey: SYZRZLUNWVNNNV-UHFFFAOYSA-N
Formula: C2H2BrClO
SMILES: O=C(Cl)CBr
Mol. weight [g/mol]: 157.39
CAS: 22118-09-8

Physical Properties

Property code	Value	Unit	Source
gf	-160.57	kJ/mol	Joback Method
hf	-186.60	kJ/mol	Joback Method
hfus	12.02	kJ/mol	Joback Method
hvap	37.61	kJ/mol	Joback Method
log10ws	-1.02		Crippen Method
logp	1.147		Crippen Method
mcvol	70.350	ml/mol	McGowan Method
pc	5782.94	kPa	Joback Method
tb	400.20	K	NIST Webbook
tb	400.00 ± 3.00	K	NIST Webbook
tc	614.35	K	Joback Method
tf	251.95	K	Joback Method
vc	0.265	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	91.80	J/mol×K	402.62	Joback Method
cpg	95.42	J/mol×K	437.91	Joback Method
cpg	98.80	J/mol×K	473.20	Joback Method
cpg	101.96	J/mol×K	508.48	Joback Method
cpg	104.89	J/mol×K	543.77	Joback Method
cpg	107.62	J/mol×K	579.06	Joback Method
cpg	110.16	J/mol×K	614.35	Joback Method

dvisc	0.0030973	Pa×s	251.95	Joback Method
dvisc	0.0020107	Pa×s	277.06	Joback Method
dvisc	0.0014024	Pa×s	302.17	Joback Method
dvisc	0.0010338	Pa×s	327.28	Joback Method
dvisc	0.0007959	Pa×s	352.40	Joback Method
dvisc	0.0006345	Pa×s	377.51	Joback Method
dvisc	0.0005203	Pa×s	402.62	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=C22118098&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
https://www.chemeo.com/cid/81-188-4/Bromoacetyl-chloride.pdf
Generated by Cheméo on 2024-04-28 11:58:09.240695936 +0000 UTC m=+16594738.161273248.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.