

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

Physical Properties

Property code	Value	Unit	Source
af	0.4044		Cheméo Relay (1.0)
gf	-160.57	kJ/mol	Joback Method
hf	-204.76	kJ/mol	Cheméo Relay (1.0)
hfus	12.02	kJ/mol	Joback Method
ie	10.57	eV	Cheméo Relay (1.0)
logp	1.147		Crippen Method
mcvol	70.350	ml/mol	McGowan Method
pc	5782.94	kPa	Joback Method
tb	400.00 ± 3.00	K	NIST Webbook
tb	400.20	K	NIST Webbook
tc	620.26	K	Cheméo Relay (1.0)
tf	317.71	K	Cheméo Relay (1.0)
vc	0.252	m3/kmol	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22118098&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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