3-BROMOPROPIONYL CHLORIDE

Other names: «beta»-Bromopropionyl chloride
Propanoyl chloride, 3-bromo-
3-Bromopropanoyl chloride
Inchi: InChI=1S/C3H4BrClO/c4-2-1-3(5)6/h1-2H2
InchiKey: IHBVNSPHKMCPST-UHFFFAOYSA-N
Formula: C3H4BrClO
SMILES: O=C(Cl)CCBr
Mol. weight [g/mol]: 171.42

Physical Properties

Property code	Value	Unit	Source
hf	-219.49	kJ/mol	Cheméo Relay (1.0)
hfus	14.61	kJ/mol	Joback Method
ie	10.34	eV	Cheméo Relay (1.0)
logp	1.537		Crippen Method
mcvol	84.440	ml/mol	McGowan Method
rinpol	913.00		NIST Webbook
tb	443.39	K	Cheméo Relay (1.0)
tf	262.13	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.76	J/mol×K	425.50	Joback Method
cpg	152.08	J/mol×K	634.89	Joback Method
cpg	148.23	J/mol×K	599.99	Joback Method
cpg	144.12	J/mol×K	565.09	Joback Method
cpg	139.73	J/mol×K	530.20	Joback Method
cpg	135.05	J/mol×K	495.30	Joback Method
cpg	130.06	J/mol×K	460.40	Joback Method
dvisc	0.0010111	Pa×s	344.36	Joback Method
dvisc	0.0004935	Pa×s	425.50	Joback Method
dvisc	0.0006068	Pa×s	398.45	Joback Method
dvisc	0.0007689	Pa×s	371.41	Joback Method

dvisc	0.0032237	Pa×s	263.22	Joback Method
dvisc	0.0013933	Pa×s	317.31	Joback Method
dvisc	0.0020381	Pa×s	290.27	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15486961&Units=SI

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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point