Methyl 2,3-bromochloropropanoate

Inchi: InChI=1S/C4H6BrClO2/c1-8-4(7)3(5)2-6/h3H,2H2,1H3
InchiKey: NEVWUGHIWINQQQ-UHFFFAOYSA-N
Formula: C4H6BrClO2
SMILES: COC(=O)C(Br)CCl
Mol. weight [g/mol]: 201.45

Physical Properties

Property code	Value	Unit	Source
gf	-251.17	kJ/mol	Joback Method
hf	-365.38	kJ/mol	Joback Method
hfus	14.86	kJ/mol	Joback Method
hvap	44.09	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	1.162		Crippen Method
mcvol	104.400	ml/mol	McGowan Method
pc	4351.13	kPa	Joback Method
rinpol	974.00		NIST Webbook
tb	470.36	K	Joback Method
tc	680.56	K	Joback Method
tf	281.72	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.47	J/mol×K	470.36	Joback Method
cpg	186.44	J/mol×K	505.39	Joback Method
cpg	193.08	J/mol×K	540.43	Joback Method
cpg	199.40	J/mol×K	575.46	Joback Method
cpg	205.38	J/mol×K	610.49	Joback Method
cpg	211.04	J/mol×K	645.53	Joback Method
cpg	216.39	J/mol×K	680.56	Joback Method
dvisc	0.0032925	Pa×s	281.72	Joback Method
dvisc	0.0018956	Pa×s	313.16	Joback Method

dvisc	0.0012070	Pa×s	344.60	Joback Method
dvisc	0.0008288	Pa×s	376.04	Joback Method
dvisc	0.0006031	Pa×s	407.48	Joback Method
dvisc	0.0004593	Pa×s	438.92	Joback Method
dvisc	0.0003628	Pa×s	470.36	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=R124999&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume