

Propanoic acid, 3-bromo-2-chloro, methyl ester

Inchi:	InChI=1S/C4H6BrClO2/c1-8-4(7)3(6)2-5/h3H,2H2,1H3
InchiKey:	XMWHGIJOJLZNQX-UHFFFAOYSA-N
Formula:	C4H6BrClO2
SMILES:	COC(=O)C(Cl)CBr
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	1024.00		NIST Webbook
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tb	470.36	K	Joback Method
tc	680.56	K	Joback Method
tf	281.72	K	Joback Method
vc	0.389	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.47	J/molxK	470.36	Joback Method
cpg	186.44	J/molxK	505.39	Joback Method
cpg	193.08	J/molxK	540.43	Joback Method
cpg	199.40	J/molxK	575.46	Joback Method
cpg	205.38	J/molxK	610.49	Joback Method
cpg	211.04	J/molxK	645.53	Joback Method
cpg	216.39	J/molxK	680.56	Joback Method
dvisc	0.0032925	Paxs	281.72	Joback Method

dvisc	0.0018956	Paxs	313.16	Joback Method
dvisc	0.0012070	Paxs	344.60	Joback Method
dvisc	0.0008288	Paxs	376.04	Joback Method
dvisc	0.0006031	Paxs	407.48	Joback Method
dvisc	0.0004593	Paxs	438.92	Joback Method
dvisc	0.0003628	Paxs	470.36	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R30321&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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