

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

Inchi:	InChI=1S/C6H10BrClO2/c1-2-3-10-6(9)5(8)4-7/h5H,2-4H2,1H3
InchiKey:	RXRSVLDNAQZHQH-UHFFFAOYSA-N
Formula:	C6H10BrClO2
SMILES:	CCCOC(=O)C(Cl)CBr
Mol. weight [g/mol]:	229.50

Physical Properties

Property code	Value	Unit	Source
gf	-234.33	kJ/mol	Joback Method
hf	-406.66	kJ/mol	Joback Method
hfus	20.04	kJ/mol	Joback Method
hvap	48.54	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.942		Crippen Method
mcvol	132.580	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
rinpol	1158.00		NIST Webbook
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tb	516.12	K	Joback Method
tc	720.33	K	Joback Method
tf	304.26	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.05	J/molxK	516.12	Joback Method
cpg	268.61	J/molxK	550.15	Joback Method
cpg	277.71	J/molxK	584.19	Joback Method
cpg	286.34	J/molxK	618.22	Joback Method
cpg	294.52	J/molxK	652.26	Joback Method
cpg	302.26	J/molxK	686.29	Joback Method
cpg	309.56	J/molxK	720.33	Joback Method
dvisc	0.0031129	Paxs	304.26	Joback Method

dvisc	0.0017190	Paxs	339.57	Joback Method
dvisc	0.0010616	Paxs	374.88	Joback Method
dvisc	0.0007123	Paxs	410.19	Joback Method
dvisc	0.0005092	Paxs	445.50	Joback Method
dvisc	0.0003823	Paxs	480.81	Joback Method
dvisc	0.0002986	Paxs	516.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R30349&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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