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

Inchi: InChI=1S/C8H14BrClO2/c1-6(2)3-4-12-8(11)7(10)5-9/h6-7H,3-5H2,1-2H3
InchiKey: JRRKUJZWCOAKNC-UHFFFAOYSA-N
Formula: C8H14BrClO2
SMILES: CC(C)CCOC(=O)C(Cl)CBr
Mol. weight [g/mol]: 257.55

Physical Properties

Property code	Value	Unit	Source
gf	-219.93	kJ/mol	Joback Method
hf	-453.22	kJ/mol	Joback Method
hfus	21.70	kJ/mol	Joback Method
hvap	52.60	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.578		Crippen Method
mcvol	160.760	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	1311.00		NIST Webbook
tb	561.44	K	Joback Method
tc	763.97	K	Joback Method
tf	311.80	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.00	J/mol×K	561.44	Joback Method
cpg	358.90	J/mol×K	595.20	Joback Method
cpg	370.18	J/mol×K	628.95	Joback Method
cpg	380.87	J/mol×K	662.71	Joback Method
cpg	390.98	J/mol×K	696.46	Joback Method
cpg	400.52	J/mol×K	730.22	Joback Method
cpg	409.50	J/mol×K	763.97	Joback Method
dvisc	0.0036916	Pa×s	311.80	Joback Method
dvisc	0.0017587	Pa×s	353.41	Joback Method

dvisc	0.0009795	Pa×s	395.01	Joback Method
dvisc	0.0006099	Pa×s	436.62	Joback Method
dvisc	0.0004124	Pa×s	478.23	Joback Method
dvisc	0.0002969	Pa×s	519.83	Joback Method
dvisc	0.0002244	Pa×s	561.44	Joback Method

Sources

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=R30264&Units=SI
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
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