Propanoic acid, 3-bromo-2-chloro, 4-methylbutyl ester

Inchi: InChI=1S/C9H16BrClO2/c1-7(2)4-3-5-13-9(12)8(11)6-10/h7-8H,3-6H2,1-2H3
InchiKey: YEKNCNQJTIFJKB-UHFFFAOYSA-N
Formula: C9H16BrClO2
SMILES: CC(C)CCCOC(=O)C(Cl)CBr
Mol. weight [g/mol]: 271.58

Physical Properties

Property code	Value	Unit	Source
gf	-211.51	kJ/mol	Joback Method
hf	-473.86	kJ/mol	Joback Method
hfus	24.29	kJ/mol	Joback Method
hvap	54.83	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.968		Crippen Method
mcvol	174.850	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
tb	584.32	K	Joback Method
tc	783.95	K	Joback Method
tf	323.07	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.53	J/mol×K	584.32	Joback Method
cpg	406.27	J/mol×K	617.59	Joback Method
cpg	418.35	J/mol×K	650.86	Joback Method
cpg	429.79	J/mol×K	684.13	Joback Method
cpg	440.60	J/mol×K	717.40	Joback Method
cpg	450.81	J/mol×K	750.68	Joback Method
cpg	460.42	J/mol×K	783.95	Joback Method
dvisc	0.0034276	Pa×s	323.07	Joback Method

dvisc	0.0016085	Pa×s	366.61	Joback Method
dvisc	0.0008864	Pa×s	410.15	Joback Method
dvisc	0.0005477	Pa×s	453.70	Joback Method
dvisc	0.0003681	Pa×s	497.24	Joback Method
dvisc	0.0002638	Pa×s	540.78	Joback Method
dvisc	0.0001987	Pa×s	584.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R30278&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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