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

Inchi: InChI=1S/C8H14BrClO2/c1-2-3-4-5-12-8(11)7(10)6-9/h7H,2-6H2,1H3
InchiKey: BJGAORWEASREFN-UHFFFAOYSA-N
Formula: C8H14BrClO2
SMILES: CCCCCOC(=O)C(Cl)CBr
Mol. weight [g/mol]: 257.55

Physical Properties

Property code	Value	Unit	Source
gf	-217.49	kJ/mol	Joback Method
hf	-447.94	kJ/mol	Joback Method
hfus	25.22	kJ/mol	Joback Method
hvap	52.99	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.722		Crippen Method
mcvol	160.760	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpol	1349.00		NIST Webbook
tb	561.88	K	Joback Method
tc	760.30	K	Joback Method
tf	326.80	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.61	J/mol×K	561.88	Joback Method
cpg	358.21	J/mol×K	594.95	Joback Method
cpg	369.23	J/mol×K	628.02	Joback Method
cpg	379.69	J/mol×K	661.09	Joback Method
cpg	389.59	J/mol×K	694.16	Joback Method
cpg	398.96	J/mol×K	727.23	Joback Method
cpg	407.80	J/mol×K	760.30	Joback Method
dvisc	0.0028158	Pa×s	326.80	Joback Method
dvisc	0.0014983	Pa×s	365.98	Joback Method

dvisc	0.0009007	Pa×s	405.16	Joback Method
dvisc	0.0005923	Pa×s	444.34	Joback Method
dvisc	0.0004169	Pa×s	483.52	Joback Method
dvisc	0.0003093	Pa×s	522.70	Joback Method
dvisc	0.0002392	Pa×s	561.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R30335&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