6-Bromohexanoic acid, 3-chloroprop-2-enyl ester

Inchi: InChI=1S/C9H14BrClO2/c10-6-3-1-2-5-9(12)13-8-4-7-11/h4,7H,1-3,5-6,8H2/b7-4+

InchiKey: UXLNBKPHAASWHX-QPJJXVBHSA-N

Formula: C9H14BrClO2

SMILES: O=C(CCCCCBr)OCC=CCl

Mol. weight [g/mol]: 269.56

Physical Properties

Property code	Value	Unit	Source
gf	-126.41	kJ/mol	Joback Method
hf	-346.08	kJ/mol	Joback Method
hfus	31.54	kJ/mol	Joback Method
hvap	55.56	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.237		Crippen Method
mcvol	170.550	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	1614.00		NIST Webbook
tb	589.36	K	Joback Method
tc	789.24	K	Joback Method
tf	347.99	K	Joback Method
vc	0.654	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.52	J/mol×K	589.36	Joback Method
cpg	384.10	J/mol×K	622.67	Joback Method
cpg	395.04	J/mol×K	655.99	Joback Method
cpg	405.39	J/mol×K	689.30	Joback Method
cpg	415.17	J/mol×K	722.62	Joback Method
cpg	424.39	J/mol×K	755.93	Joback Method
cpg	433.10	J/mol×K	789.24	Joback Method
dvisc	0.0019437	Pa×s	347.99	Joback Method
dvisc	0.0010848	Pa×s	388.22	Joback Method

dvisc	0.0006755	Pa×s	428.45	Joback Method
dvisc	0.0004563	Pa×s	468.68	Joback Method
dvisc	0.0003279	Pa×s	508.90	Joback Method
dvisc	0.0002474	Pa×s	549.13	Joback Method
dvisc	0.0001939	Pa×s	589.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299296&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