

4-Bromobutanoic acid, 3-chloroprop-2-enyl ester

Inchi:	InChI=1S/C7H10BrClO2/c8-4-1-3-7(10)11-6-2-5-9/h2,5H,1,3-4,6H2/b5-2+
InchiKey:	MXEQMDIIUFQSMS-GORDUTHDSA-N
Formula:	C7H10BrClO2
SMILES:	O=C(CCCBr)OCC=CCl
Mol. weight [g/mol]:	241.51

Physical Properties

Property code	Value	Unit	Source
gf	-143.25	kJ/mol	Joback Method
hf	-304.80	kJ/mol	Joback Method
hfus	26.36	kJ/mol	Joback Method
hvap	51.11	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.457		Crippen Method
mvol	142.370	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	1391.00		NIST Webbook
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tb	543.60	K	Joback Method
tc	749.48	K	Joback Method
tf	325.45	K	Joback Method
vc	0.542	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.41	J/molxK	543.60	Joback Method
cpg	292.15	J/molxK	577.91	Joback Method
cpg	301.35	J/molxK	612.23	Joback Method
cpg	310.02	J/molxK	646.54	Joback Method
cpg	318.20	J/molxK	680.86	Joback Method
cpg	325.91	J/molxK	715.17	Joback Method
cpg	333.16	J/molxK	749.48	Joback Method
dvisc	0.0021465	Paxs	325.45	Joback Method

dvisc	0.0012427	Paxs	361.81	Joback Method
dvisc	0.0007949	Paxs	398.17	Joback Method
dvisc	0.0005480	Paxs	434.52	Joback Method
dvisc	0.0004001	Paxs	470.88	Joback Method
dvisc	0.0003056	Paxs	507.24	Joback Method
dvisc	0.0002420	Paxs	543.60	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=U299285&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

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