

5-Bromovaleric acid, 3-chloroprop-2-enyl ester

Inchi:	InChI=1S/C8H12BrClO2/c9-5-2-1-4-8(11)12-7-3-6-10/h3,6H,1-2,4-5,7H2/b6-3+
InchiKey:	WKBNROJJOCKZAN-ZZXKWWIFSA-N
Formula:	C8H12BrClO2
SMILES:	O=C(CCCCBBr)OCC=CCl
Mol. weight [g/mol]:	255.54

Physical Properties

Property code	Value	Unit	Source
gf	-134.83	kJ/mol	Joback Method
hf	-325.44	kJ/mol	Joback Method
hfus	28.95	kJ/mol	Joback Method
hvap	53.34	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.847		Crippen Method
mcvol	156.460	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	1567.60		NIST Webbook
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tb	566.48	K	Joback Method
tc	769.28	K	Joback Method
tf	336.72	K	Joback Method
vc	0.599	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.58	J/molxK	566.48	Joback Method
cpg	337.30	J/molxK	600.28	Joback Method
cpg	347.42	J/molxK	634.08	Joback Method
cpg	356.99	J/molxK	667.88	Joback Method
cpg	366.01	J/molxK	701.68	Joback Method
cpg	374.52	J/molxK	735.48	Joback Method
cpg	382.55	J/molxK	769.28	Joback Method
dvisc	0.0020522	Paxs	336.72	Joback Method

dvisc	0.0011659	Paxs	375.01	Joback Method
dvisc	0.0007356	Paxs	413.31	Joback Method
dvisc	0.0005018	Paxs	451.60	Joback Method
dvisc	0.0003634	Paxs	489.89	Joback Method
dvisc	0.0002758	Paxs	528.19	Joback Method
dvisc	0.0002172	Paxs	566.48	Joback Method

Sources

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=U292571&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	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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