

2-(2-Chloroethoxy)-3-methyl-1-butene

Inchi:	InChI=1S/C7H13ClO/c1-6(2)7(3)9-5-4-8/h6H,3-5H2,1-2H3
InchiKey:	JBPGDBXWROOKKP-UHFFFAOYSA-N
Formula:	C7H13ClO
SMILES:	C=C(OCCCl)C(C)C
Mol. weight [g/mol]:	148.63
CAS:	56798-14-2

Physical Properties

Property code	Value	Unit	Source
gf	-32.02	kJ/mol	Joback Method
hf	-225.41	kJ/mol	Joback Method
hfus	13.16	kJ/mol	Joback Method
hvap	36.99	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	2.412		Crippen Method
mcvol	123.300	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
tb	415.53	K	Joback Method
tc	598.36	K	Joback Method
tf	190.08	K	Joback Method
vc	0.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.47	J/mol×K	415.53	Joback Method
cpg	242.72	J/mol×K	446.00	Joback Method
cpg	253.54	J/mol×K	476.47	Joback Method
cpg	263.93	J/mol×K	506.95	Joback Method
cpg	273.90	J/mol×K	537.42	Joback Method
cpg	283.46	J/mol×K	567.89	Joback Method
cpg	292.61	J/mol×K	598.36	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C56798142&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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