

2-Butene, 2-(2-chloroethoxy)-3-methyl-

Inchi:	InChI=1S/C7H13ClO/c1-6(2)7(3)9-5-4-8/h4-5H2,1-3H3
InchiKey:	HAACTQJIKFKSSS-UHFFFAOYSA-N
Formula:	C7H13ClO
SMILES:	CC(C)=C(C)OCCCl
Mol. weight [g/mol]:	148.63
CAS:	56798-15-3

Physical Properties

Property code	Value	Unit	Source
gf	-45.75	kJ/mol	Joback Method
hf	-238.13	kJ/mol	Joback Method
hfus	16.85	kJ/mol	Joback Method
hvap	38.09	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.556		Crippen Method
mcvol	123.300	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	423.33	K	Joback Method
tc	610.77	K	Joback Method
tf	187.80	K	Joback Method
vc	0.476	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.29	J/mol×K	423.33	Joback Method
cpg	242.71	J/mol×K	454.57	Joback Method
cpg	253.64	J/mol×K	485.81	Joback Method
cpg	264.09	J/mol×K	517.05	Joback Method
cpg	274.09	J/mol×K	548.29	Joback Method
cpg	283.65	J/mol×K	579.53	Joback Method
cpg	292.77	J/mol×K	610.77	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C56798153&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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