2-Chloromethoxy-3-chloro-tetrahydro-furan

Other names: Tetrahydrofuran, 3-chloro-2-chloromethoxy
Inchi: InChI=1S/C5H8Cl2O2/c6-3-9-5-4(7)1-2-8-5/h4-5H,1-3H2
InchiKey: KXPHIXYZKVEVPV-UHFFFAOYSA-N
Formula: C5H8Cl2O2
SMILES: ClCOC1OCCC1Cl
Mol. weight [g/mol]: 171.02

Physical Properties

Property code	Value	Unit	Source
gf	-194.92	kJ/mol	Joback Method
hf	-402.09	kJ/mol	Joback Method
hfus	21.27	kJ/mol	Joback Method
hvap	42.36	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.553		Crippen Method
mcvol	106.670	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
rinpol	1085.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1085.00		NIST Webbook
tb	448.64	K	Joback Method
tc	661.01	K	Joback Method
tf	261.41	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.56	J/mol×K	448.64	Joback Method
cpg	215.90	J/mol×K	484.03	Joback Method
cpg	226.70	J/mol×K	519.43	Joback Method
cpg	236.96	J/mol×K	554.82	Joback Method
cpg	246.70	J/mol×K	590.22	Joback Method
cpg	255.90	J/mol×K	625.61	Joback Method

cpg	264.57	J/mol×K	661.01	Joback Method
dvisc	0.0025432	Pa×s	261.41	Joback Method
dvisc	0.0015999	Pa×s	292.61	Joback Method
dvisc	0.0011006	Pa×s	323.82	Joback Method
dvisc	0.0008085	Pa×s	355.02	Joback Method
dvisc	0.0006243	Pa×s	386.23	Joback Method
dvisc	0.0005011	Pa×s	417.43	Joback Method
dvisc	0.0004147	Pa×s	448.64	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R91294&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

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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