1-chlorobutyl chloroacetate

Other names: 1-Butanol, 1-chloro, chloroacetate
Inchi: InChI=1S/C6H10Cl2O2/c1-2-3-5(8)10-6(9)4-7/h5H,2-4H2,1H3
InchiKey: KXHRHLNXCBLCOB-UHFFFAOYSA-N
Formula: C6H10Cl2O2
SMILES: CCCC(Cl)OC(=O)CCl
Mol. weight [g/mol]: 185.05

Physical Properties

Property code	Value	Unit	Source
gf	-260.58	kJ/mol	Joback Method
hf	-448.73	kJ/mol	Joback Method
hfus	18.95	kJ/mol	Joback Method
hvap	46.49	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.133		Crippen Method
mcvol	127.320	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	1106.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1102.00		NIST Webbook
ripol	1674.00		NIST Webbook
ripol	1701.00		NIST Webbook
ripol	1701.00		NIST Webbook
ripol	1701.00		NIST Webbook
ripol	1709.00		NIST Webbook
ripol	1674.00		NIST Webbook
ripol	1709.00		NIST Webbook
ripol	1669.00		NIST Webbook
tb	487.39	K	Joback Method
tc	681.93	K	Joback Method
tf	274.38	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.20	J/mol×K	487.39	Joback Method
cpg	258.74	J/mol×K	519.81	Joback Method
cpg	267.87	J/mol×K	552.24	Joback Method
cpg	276.59	J/mol×K	584.66	Joback Method
cpg	284.91	J/mol×K	617.08	Joback Method
cpg	292.82	J/mol×K	649.50	Joback Method
cpg	300.33	J/mol×K	681.93	Joback Method
dvisc	0.0038678	Pa×s	274.38	Joback Method
dvisc	0.0019631	Pa×s	309.88	Joback Method
dvisc	0.0011455	Pa×s	345.38	Joback Method
dvisc	0.0007390	Pa×s	380.88	Joback Method
dvisc	0.0005137	Pa×s	416.39	Joback Method
dvisc	0.0003781	Pa×s	451.89	Joback Method
dvisc	0.0002910	Pa×s	487.39	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R111512&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume