4-chlorobutyl chloroacetate

Other names: 1-Butanol, 4-chloro, chloroacetate
Inchi: InChI=1S/C6H10Cl2O2/c7-3-1-2-4-10-6(9)5-8/h1-5H2
InchiKey: DQLULOGYMQTGQE-UHFFFAOYSA-N
Formula: C6H10Cl2O2
SMILES: O=C(CCl)OCCCCCl
Mol. weight [g/mol]: 185.05

Physical Properties

Property code	Value	Unit	Source
gf	-258.14	kJ/mol	Joback Method
hf	-443.45	kJ/mol	Joback Method
hfus	22.48	kJ/mol	Joback Method
hvap	46.88	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.787		Crippen Method
mcvol	127.320	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
rinpol	1251.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1247.00		NIST Webbook
ripol	2036.00		NIST Webbook
ripol	2028.00		NIST Webbook
ripol	2017.00		NIST Webbook
ripol	2010.00		NIST Webbook
ripol	1968.00		NIST Webbook
tb	487.83	K	Joback Method
tc	678.17	K	Joback Method
tf	289.38	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	248.95	J/mol×K	487.83	Joback Method
cpg	291.42	J/mol×K	646.44	Joback Method
cpg	283.68	J/mol×K	614.72	Joback Method
cpg	275.57	J/mol×K	583.00	Joback Method
cpg	267.08	J/mol×K	551.28	Joback Method
cpg	258.21	J/mol×K	519.55	Joback Method
cpg	298.78	J/mol×K	678.17	Joback Method
dvisc	0.0003070	Pa×s	487.83	Joback Method
dvisc	0.0003889	Pa×s	454.75	Joback Method
dvisc	0.0005113	Pa×s	421.68	Joback Method
dvisc	0.0007043	Pa×s	388.61	Joback Method
dvisc	0.0010297	Pa×s	355.53	Joback Method
dvisc	0.0016272	Pa×s	322.45	Joback Method
dvisc	0.0028553	Pa×s	289.38	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=R111601&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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