3-chlorobutyl dichloroacetate

Other names: 1-Butanol, 3-chloro, dichloroacetate
Inchi: InChI=1S/C6H9Cl3O2/c1-4(7)2-3-11-6(10)5(8)9/h4-5H,2-3H2,1H3
InchiKey: WOMWKYYCERCSDL-UHFFFAOYSA-N
Formula: C6H9Cl3O2
SMILES: CC(Cl)CCOC(=O)C(Cl)Cl
Mol. weight [g/mol]: 219.49

Physical Properties

Property code	Value	Unit	Source
gf	-274.95	kJ/mol	Joback Method
hf	-469.75	kJ/mol	Joback Method
hfus	19.63	kJ/mol	Joback Method
hvap	50.48	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.351		Crippen Method
mcvol	139.560	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
rinpol	1252.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1231.00		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1961.00		NIST Webbook
ripol	1906.00		NIST Webbook
ripol	1939.00		NIST Webbook
ripol	1942.00		NIST Webbook
tb	524.38	K	Joback Method
tc	728.53	K	Joback Method
tf	289.30	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.66	J/mol×K	524.38	Joback Method
cpg	281.98	J/mol×K	558.41	Joback Method
cpg	290.84	J/mol×K	592.43	Joback Method
cpg	299.23	J/mol×K	626.46	Joback Method
cpg	307.16	J/mol×K	660.48	Joback Method
cpg	314.64	J/mol×K	694.51	Joback Method
cpg	321.66	J/mol×K	728.53	Joback Method
dvisc	0.0045405	Pa×s	289.30	Joback Method
dvisc	0.0021323	Pa×s	328.48	Joback Method
dvisc	0.0011764	Pa×s	367.66	Joback Method
dvisc	0.0007278	Pa×s	406.84	Joback Method
dvisc	0.0004899	Pa×s	446.02	Joback Method
dvisc	0.0003515	Pa×s	485.20	Joback Method
dvisc	0.0002651	Pa×s	524.38	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=R111587&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