4-chlorobutyl dichloroacetate

Other names: 1-Butanol, 4-chloro, dichloroacetate
Inchi: InChI=1S/C6H9Cl3O2/c7-3-1-2-4-11-6(10)5(8)9/h5H,1-4H2
InchiKey: QBXNHPCFNUVPAE-UHFFFAOYSA-N
Formula: C6H9Cl3O2
SMILES: O=C(OCCCCCl)C(Cl)Cl
Mol. weight [g/mol]: 219.49

Physical Properties

Property code	Value	Unit	Source
gf	-272.51	kJ/mol	Joback Method
hf	-464.47	kJ/mol	Joback Method
hfus	23.15	kJ/mol	Joback Method
hvap	50.87	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.352		Crippen Method
mcvol	139.560	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
rinpol	1325.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1332.00		NIST Webbook
ripol	2106.00		NIST Webbook
ripol	2083.00		NIST Webbook
ripol	2076.00		NIST Webbook
ripol	2097.00		NIST Webbook
ripol	2044.00		NIST Webbook
tb	524.82	K	Joback Method
tc	724.62	K	Joback Method
tf	304.30	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.31	J/mol×K	524.82	Joback Method
cpg	313.24	J/mol×K	691.32	Joback Method
cpg	305.92	J/mol×K	658.02	Joback Method
cpg	298.17	J/mol×K	624.72	Joback Method
cpg	289.98	J/mol×K	591.42	Joback Method
cpg	281.37	J/mol×K	558.12	Joback Method
cpg	320.14	J/mol×K	724.62	Joback Method
dvisc	0.0002812	Pa×s	524.82	Joback Method
dvisc	0.0003638	Pa×s	488.07	Joback Method
dvisc	0.0004909	Pa×s	451.31	Joback Method
dvisc	0.0006984	Pa×s	414.56	Joback Method
dvisc	0.0010644	Pa×s	377.81	Joback Method
dvisc	0.0017763	Pa×s	341.05	Joback Method
dvisc	0.0033548	Pa×s	304.30	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=R111616&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