3-chlorobutyl trichloroacetate

Other names: 1-Butanol, 3-chloro, trichloroacetate
Inchi: InChI=1S/C6H8Cl4O2/c1-4(7)2-3-12-5(11)6(8,9)10/h4H,2-3H2,1H3
InchiKey: NAGGOAXMLNBTCJ-UHFFFAOYSA-N
Formula: C6H8Cl4O2
SMILES: CC(Cl)CCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 253.94

Physical Properties

Property code	Value	Unit	Source
gf	-281.60	kJ/mol	Joback Method
hf	-488.96	kJ/mol	Joback Method
hfus	19.93	kJ/mol	Joback Method
hvap	53.96	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.917		Crippen Method
mcvol	151.800	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	1337.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1289.00		NIST Webbook
ripol	1875.00		NIST Webbook
ripol	1941.00		NIST Webbook
ripol	1923.00		NIST Webbook
ripol	1911.00		NIST Webbook
ripol	1900.00		NIST Webbook
ripol	1875.00		NIST Webbook
tb	559.02	K	Joback Method
tc	776.12	K	Joback Method
tf	336.64	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.23	J/mol×K	559.02	Joback Method
cpg	307.26	J/mol×K	595.20	Joback Method
cpg	315.65	J/mol×K	631.39	Joback Method
cpg	323.42	J/mol×K	667.57	Joback Method
cpg	330.62	J/mol×K	703.76	Joback Method
cpg	337.27	J/mol×K	739.94	Joback Method
cpg	343.39	J/mol×K	776.12	Joback Method
dvisc	0.0032699	Pa×s	336.64	Joback Method
dvisc	0.0017065	Pa×s	373.70	Joback Method
dvisc	0.0010015	Pa×s	410.77	Joback Method
dvisc	0.0006420	Pa×s	447.83	Joback Method
dvisc	0.0004404	Pa×s	484.89	Joback Method
dvisc	0.0003188	Pa×s	521.96	Joback Method
dvisc	0.0002408	Pa×s	559.02	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=R111592&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