4-chlorobutyl trichloroacetate

Other names: 1-Butanol, 4-chloro, trichloroacetate
Inchi: InChI=1S/C6H8Cl4O2/c7-3-1-2-4-12-5(11)6(8,9)10/h1-4H2
InchiKey: JMIOMLKQYQMROM-UHFFFAOYSA-N
Formula: C6H8Cl4O2
SMILES: O=C(OCCCCCl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 253.94

Physical Properties

Property code	Value	Unit	Source
gf	-279.16	kJ/mol	Joback Method
hf	-483.68	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	54.35	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.919		Crippen Method
mcvol	151.800	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
rinpol	1364.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1365.00		NIST Webbook
ripol	2023.00		NIST Webbook
ripol	2079.00		NIST Webbook
ripol	2093.00		NIST Webbook
ripol	2023.00		NIST Webbook
ripol	2061.00		NIST Webbook
ripol	2050.00		NIST Webbook
tb	559.46	K	Joback Method
tc	771.93	K	Joback Method
tf	351.64	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.80	J/mol×K	559.46	Joback Method
cpg	335.92	J/mol×K	736.52	Joback Method
cpg	329.39	J/mol×K	701.11	Joback Method
cpg	322.34	J/mol×K	665.70	Joback Method
cpg	314.75	J/mol×K	630.28	Joback Method
cpg	306.58	J/mol×K	594.87	Joback Method
cpg	341.96	J/mol×K	771.93	Joback Method
dvisc	0.0002566	Pa×s	559.46	Joback Method
dvisc	0.0003314	Pa×s	524.82	Joback Method
dvisc	0.0004438	Pa×s	490.19	Joback Method
dvisc	0.0006214	Pa×s	455.55	Joback Method
dvisc	0.0009195	Pa×s	420.91	Joback Method
dvisc	0.0014598	Pa×s	386.28	Joback Method
dvisc	0.0025384	Pa×s	351.64	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=R111621&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

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