

4-Chlorobutyric acid, 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C6H8Cl4O2/c7-3-1-2-5(11)12-4-6(8,9)10/h1-4H2
InchiKey: GIEQAPHJNYGVAX-UHFFFAOYSA-N
Formula: C6H8Cl4O2
SMILES: O=C(CCCCl)OCC(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	1450.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1466.00		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/molxK	559.46	Joback Method
cpg	306.58	J/molxK	594.87	Joback Method
cpg	314.75	J/molxK	630.28	Joback Method
cpg	322.34	J/molxK	665.70	Joback Method
cpg	329.39	J/molxK	701.11	Joback Method
cpg	335.92	J/molxK	736.52	Joback Method
cpg	341.96	J/molxK	771.93	Joback Method

dvisc	0.0025384	Paxs	351.64	Joback Method
dvisc	0.0014598	Paxs	386.28	Joback Method
dvisc	0.0009195	Paxs	420.91	Joback Method
dvisc	0.0006214	Paxs	455.55	Joback Method
dvisc	0.0004438	Paxs	490.19	Joback Method
dvisc	0.0003314	Paxs	524.82	Joback Method
dvisc	0.0002566	Paxs	559.46	Joback Method

Sources

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=U360640&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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