

Carbonochloridic acid, 3-chloropropyl ester

Other names:	Formic acid, chloro-, 3-chloropropyl ester (3-Chloropropoxy)carbonyl chloride 3-Chloropropyl chloroformate 3-Chloropropyl chloridocarbonate
Inchi:	InChI=1S/C4H6Cl2O2/c5-2-1-3-8-4(6)7/h1-3H2
InchiKey:	MTXMEFUEBCFWCY-UHFFFAOYSA-N
Formula:	C4H6Cl2O2
SMILES:	O=C(Cl)OCCCl
Mol. weight [g/mol]:	157.00
CAS:	628-11-5

Physical Properties

Property code	Value	Unit	Source
gf	-274.98	kJ/mol	Joback Method
hf	-402.17	kJ/mol	Joback Method
hfus	17.30	kJ/mol	Joback Method
hvap	42.42	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.991		Crippen Method
mcvol	99.140	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
rinpol	999.00		NIST Webbook
tb	442.07	K	Joback Method
tc	636.71	K	Joback Method
tf	266.84	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.94	J/molxK	442.07	Joback Method
cpg	178.56	J/molxK	474.51	Joback Method
cpg	184.93	J/molxK	506.95	Joback Method
cpg	191.05	J/molxK	539.39	Joback Method

cpg	196.92	J/molxK	571.83	Joback Method
cpg	202.53	J/molxK	604.27	Joback Method
cpg	207.89	J/molxK	636.71	Joback Method
dvisc	0.0028294	Paxs	266.84	Joback Method
dvisc	0.0016875	Paxs	296.05	Joback Method
dvisc	0.0011043	Paxs	325.25	Joback Method
dvisc	0.0007750	Paxs	354.46	Joback Method
dvisc	0.0005740	Paxs	383.66	Joback Method
dvisc	0.0004436	Paxs	412.87	Joback Method
dvisc	0.0003546	Paxs	442.07	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=C628115&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
mcvol:	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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