

Cyclopropanecarboxylic acid chloride

Other names:	Cyclopropane carbonyl chloride Cyclopropylcarboxyl chloride
Inchi:	InChI=1S/C4H5ClO/c5-4(6)3-1-2-3/h3H,1-2H2
InchiKey:	ZOOSILUVXHVRJE-UHFFFAOYSA-N
Formula:	C4H5ClO
SMILES:	O=C(Cl)C1CC1
Mol. weight [g/mol]:	104.53
CAS:	4023-34-1

Physical Properties

Property code	Value	Unit	Source
gf	-97.30	kJ/mol	Joback Method
hf	-181.41	kJ/mol	Joback Method
hfus	10.05	kJ/mol	Joback Method
hvap	35.54	kJ/mol	Joback Method
log10ws	-1.08		Crippen Method
logp	1.162		Crippen Method
mcvol	70.170	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
tb	392.20	K	NIST Webbook
tb	390.00 ± 2.00	K	NIST Webbook
tc	593.50	K	Joback Method
tf	232.63	K	Joback Method
vc	0.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.08	J/mol×K	388.96	Joback Method
cpg	122.37	J/mol×K	423.05	Joback Method
cpg	130.09	J/mol×K	457.14	Joback Method
cpg	137.28	J/mol×K	491.23	Joback Method
cpg	143.96	J/mol×K	525.32	Joback Method
cpg	150.18	J/mol×K	559.41	Joback Method

cpg	155.96	J/mol×K	593.50	Joback Method
dvisc	0.0014581	Pa×s	232.63	Joback Method
dvisc	0.0011300	Pa×s	258.69	Joback Method
dvisc	0.0009176	Pa×s	284.74	Joback Method
dvisc	0.0007715	Pa×s	310.79	Joback Method
dvisc	0.0006664	Pa×s	336.85	Joback Method
dvisc	0.0005878	Pa×s	362.90	Joback Method
dvisc	0.0005273	Pa×s	388.96	Joback Method

Sources

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=C4023341&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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