

Cyclobutanecarboxylic acid chloride

Other names:	Cyclobutanecarbonyl chloride Cyclobutane carboxyl chloride
Inchi:	InChI=1S/C5H7ClO/c6-5(7)4-2-1-3-4/h4H,1-3H2
InchiKey:	JFWMYCVMQSLLOO-UHFFFAOYSA-N
Formula:	C5H7ClO
SMILES:	O=C(Cl)C1CCC1
Mol. weight [g/mol]:	118.56
CAS:	5006-22-4

Physical Properties

Property code	Value	Unit	Source
gf	-100.98	kJ/mol	Joback Method
hf	-208.21	kJ/mol	Joback Method
hfus	10.54	kJ/mol	Joback Method
hvap	37.94	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.552		Crippen Method
mvol	84.260	ml/mol	McGowan Method
pc	4345.39	kPa	Joback Method
tb	409.00 ± 3.00	K	NIST Webbook
tc	627.33	K	Joback Method
tf	240.38	K	Joback Method
vc	0.320	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.55	J/mol×K	416.11	Joback Method
cpg	193.73	J/mol×K	592.13	Joback Method
cpg	185.68	J/mol×K	556.93	Joback Method
cpg	177.07	J/mol×K	521.72	Joback Method
cpg	167.87	J/mol×K	486.52	Joback Method
cpg	158.04	J/mol×K	451.31	Joback Method
cpg	201.24	J/mol×K	627.33	Joback Method

dvisc	0.0005108	Paxs	416.11	Joback Method
dvisc	0.0006012	Paxs	386.82	Joback Method
dvisc	0.0007269	Paxs	357.53	Joback Method
dvisc	0.0009091	Paxs	328.25	Joback Method
dvisc	0.0011879	Paxs	298.96	Joback Method
dvisc	0.0016452	Paxs	269.67	Joback Method
dvisc	0.0024665	Paxs	240.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.20	K	6.70	NIST Webbook

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=C5006224&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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

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