

2-Furancarboxyl chloride

Other names:	2-Furoyl chloride «alpha»-Furoic chloride Furan-2-carboxyl chloride Furan, 2-(chloroformyl)- Pyromucyl chloride 2-(Chloroformyl)furan 2-Chlorocarboxylfuran 2-Furancarboxylic acid chloride
Inchi:	InChI=1S/C5H3ClO2/c6-5(7)4-2-1-3-8-4/h1-3H
InchiKey:	OFTKFKYVSBNYEC-UHFFFAOYSA-N
Formula:	C5H3ClO2
SMILES:	O=C(Cl)c1ccco1
Mol. weight [g/mol]:	130.53
CAS:	527-69-5

Physical Properties

Property code	Value	Unit	Source
ie	9.44	eV	NIST Webbook
ie	9.56	eV	NIST Webbook
log10ws	-6.10		Crippen Method
logp	1.659		Crippen Method
mcvol	81.530	ml/mol	McGowan Method
tb	446.20	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	339.20	K	1.30	NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C527695&Units=SI>

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

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