

Thianaphthene-2-carbonyl chloride

Other names:	Benzo[b]thiophene-2-carbonyl chloride
Inchi:	InChI=1S/C9H5ClOS/c10-9(11)8-5-6-3-1-2-4-7(6)12-8/h1-5H
InchiKey:	DNGLRCHMGDDHNC-UHFFFAOYSA-N
Formula:	C9H5ClOS
SMILES:	O=C(Cl)c1cc2ccccc2s1
Mol. weight [g/mol]:	196.65
CAS:	39827-11-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.92		Crippen Method
logp	3.280		Crippen Method
mccvol	128.910	ml/mol	McGowan Method
tf	361.50 ± 0.50	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	447.00 ± 1.00	K	2.50	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=C39827117&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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