

Ethanone,2,2,2-trifluoro-1-(2-thienyl)-

Other names:	2-(Trifluoroacetyl)thiophene
Inchi:	InChI=1S/C6H3F3OS/c7-6(8,9)5(10)4-2-1-3-11-4/h1-3H
InchiKey:	CZYKJGCKVBXLGF-UHFFFAOYSA-N
Formula:	C6H3F3OS
SMILES:	O=C(c1cccs1)C(F)(F)F
Mol. weight [g/mol]:	180.15
CAS:	651-70-7

Physical Properties

Property code	Value	Unit	Source
ie	9.70 ± 0.05	eV	NIST Webbook
log10ws	-2.55		Crippen Method
logp	2.493		Crippen Method
mcvol	99.170	ml/mol	McGowan Method

Sources

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=C651707&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/68-792-8/Ethanone-2-2-2-trifluoro-1-2-thienyl.pdf>

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