

9H-Thioxanthen-9-one, 2-(trifluoromethyl)-

Other names:	2-(Trifluoromethyl)thioxanthen-9-one 2-(trifluoromethyl)-9H-thioxanthen-9-one
Inchi:	InChI=1S/C14H7F3OS/c15-14(16,17)8-5-6-12-10(7-8)13(18)9-3-1-2-4-11(9)19-12/h1-7H
InchiKey:	NEWRXGDGZGIHIS-UHFFFAOYSA-N
Formula:	C14H7F3OS
SMILES:	O=c1c2ccccc2sc2ccc(C(F)(F)F)cc12
Mol. weight [g/mol]:	280.26
CAS:	1693-28-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.36		Crippen Method
logp	4.434		Crippen Method
mcvol	172.970	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=C1693283&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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/92-714-7/9H-Thioxanthen-9-one-2-trifluoromethyl.pdf>

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