DITHIOPYR

Other names:	Dimethyl 2-(difluoromethyl)-4-isobutyl-6-(trifluoromethyl)pyridine-3,5-dicarbothioate 3,5-Pyridinedicarbothioic acid, 2-(difluoromethyl)-4-(2-methylpropyl)-6-(trifluoromethyl)-, 3,5-dimethyl ester
Inchi:	InChI=1S/C15H16F5NO2S2/c1-6(2)5-7-8(13(22)24-3)10(12(16)17)21-11(15(18,19)20)9(
InchiKey:	YUBJPYNSGLJZPQ-UHFFFAOYSA-N
Formula:	C15H16F5NO2S2
SMILES:	CSC(=O)c1c(C(F)F)nc(C(F)(F)F)c(C(=O)SC)c1CC(C)C
Mol. weight [g/mol]:	401.42
CAS:	97886-45-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.86		Crippen Method
logp	5.243		Crippen Method
mcvol	253.120	ml/mol	McGowan Method
rinpol	1920.00		NIST Webbook
rinpol	1925.00		NIST Webbook
rinpol	1893.00		NIST Webbook
rinpol	1958.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1893.00		NIST Webbook

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=C97886458&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices