

Thifluzamide

Other names: 5-Thiazolecarboxamide,
Inchi: N-[2,6-dibromo-4-(trifluoromethoxy)phenyl]-2-methyl-4-(trifluoromethyl)-
InchiKey: WOSNCVAPUOFXEH-UHFFFAOYSA-N
Formula: C₁₃H₆Br₂F₆N₂O₂S
SMILES: Cc1nc(C(F)(F)F)c(C(=O)Nc2c(Br)cc(OC(F)(F)F)cc2Br)s1
Mol. weight [g/mol]: 528.06
CAS: 130000-40-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.15		Crippen Method
logp	6.146		Crippen Method
mcvol	240.180	ml/mol	McGowan Method
rinpol	2190.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C130000407&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/22-388-7/Thifluzamide.pdf>

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