

Benzenamine, N-[3-phenyl-4,5-bis[(trifluoromethyl)imino]-2-thiaz

Other names:

BAY SLJ 0312

Cropotex

Flubenzimine

N-(3-Phenyl-4,5-bis((trifluoromethyl)imino)-2-thiazolidinylidene)benzenamine

SLJ 0312

Flubenzimin

N-[3-phenyl-4,5-bis[(trifluoromethyl)imino]thiazolidin-2-ylidene]aniline

Inchi: InChI=1S/C17H10F6N4S/c18-16(19,20)25-13-14(26-17(21,22)23)28-15(24-11-7-3-1-4-8

InchiKey: IZFZCMFMJKDHJZ-UHFFFAOYSA-N

Formula: C17H10F6N4S

SMILES: FC(F)(F)N=C1SC(=Nc2ccccc2)N(c2ccccc2)C1=NC(F)(F)F

Mol. weight [g/mol]: 416.34

CAS: 37893-02-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.42		Crippen Method
logp	5.764		Crippen Method
mvol	246.000	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C37893020&Units=SI>

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>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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