

Trimetozine

Other names:

Morpholine, 4-(3,4,5-trimethoxybenzoyl)-
PS-2383
Sedoxazine
Trifenoxazin
Trimethoxazine
4-(3,4,5-Trimethoxybenzoyl)morpholine
N-(3,4,5-Trimethoxybenzoyl)tetrahydro-1,4-oxazine
4-(3,4,5-Trimethoxybenzoyl)tetrahydro-1,4-oxazine
3,4,5-Trimethoxybenzoyl-N-tetrahydroxazine
Trimetozin
Trioxazin
Trioxazine
A 22370
Abbott-22370
LG 50043
N-(3,4,5-Trimethoxybenzoyl)morpholine
Opalene
Triksazin
Trimetogine
Trimetozina
V 7
3,4,5-Trimethoxy-N-benzoyltetrahydroxazine
NSC-62939
Trimolide

Inchi: InChI=1S/C14H19NO5/c1-17-11-8-10(9-12(18-2)13(11)19-3)14(16)15-4-6-20-7-5-15/h8-9
InchiKey: XWVOEFLBOSSYGM-UHFFFAOYSA-N
Formula: C14H19NO5
SMILES: COc1cc(C(=O)N2CCOCC2)cc(OC)c1OC
Mol. weight [g/mol]: 281.30
CAS: 635-41-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.79		Crippen Method
logp	1.185		Crippen Method
mccvol	208.530	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=C635416&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

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