

Tinidazole

Inchi:	InChI=1S/C8H13N3O4S/c1-3-16(14,15)5-4-10-7(2)9-6-8(10)11(12)13/h6H,3-5H2,1-2H3
InchiKey:	HJLSLZFTENLFI-UHFFFAOYSA-N
Formula:	C8H13N3O4S
SMILES:	CCS(=O)(=O)CCn1c([N+](=O)[O-])cnc1C
Mol. weight [g/mol]:	247.28
CAS:	19387-91-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Cheméo Relay (1.0)
logp	0.534		Crippen Method
mcvol	169.590	ml/mol	McGowan Method
tf	400.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting
Point Dataset (2014, CC0):
McGowan Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/112-549-8/Tinidazole.pdf>

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