Ticrynafen

Inchi: InChI=1S/C13H8Cl2O4S/c14-11-7(13(18)9-2-1-5-20-9)3-4-8(12(11)15)19-6-10(16)17/h1-

InchiKey: AGHANLSBXUWXTB-UHFFFAOYSA-N

Formula: C13H8Cl2O4S

SMILES: O=C(O)COc1ccc(C(=O)c2cccs2)c(Cl)c1Cl

Mol. weight [g/mol]: 331.18

CAS: 40180-04-9

Physical Properties

Property code	Value	Unit	Source
ie	8.59	eV	Cheméo Relay (1.0)
log10ws	-4.28		Cheméo Relay (1.0)
logp	3.749		Crippen Method
mcvol	206.520	ml/mol	McGowan Method
tb	666.54	K	Cheméo Relay (1.0)
tf	422.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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