Chlorimuron ethyl

Inchi: InChI=1S/C15H15ClN4O6S/c1-3-26-13(21)9-6-4-5-7-10(9)27(23,24)20-15(22)19-14-17-12(16)8-11(25-2)18-14/h4-8H,3H2,1-2H3,(H2,17,18,19,20,22)

InchiKey: NSWAMPCUPHPTTC-UHFFFAOYSA-N

Formula: C15H15ClN4O6S

SMILES: CCOC(=O)c1ccccc1S(=O)(=O)NC(=O)Nc1nc(Cl)cc(OC)n1

Mol. weight [g/mol]: 414.83

CAS: 90982-32-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.62		Cheméo Relay (1.0)
logp	1.826		Crippen Method
mcvol	269.820	ml/mol	McGowan Method
tb	696.73	K	Cheméo Relay (1.0)
tf	454.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

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

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):

Legend

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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