

Triasulfuron

Inchi:	InChI=1S/C14H16ClN5O5S/c1-9-16-12(19-14(17-9)24-2)18-13(21)20-26(22,23)11-6-4-3
InchiKey:	XOPFESVZMSQIKC-UHFFFAOYSA-N
Formula:	C14H16ClN5O5S
SMILES:	<chem>COc1nc(C)nc(NC(=O)NS(=O)(=O)c2ccccc2OCCCl)n1</chem>
Mol. weight [g/mol]:	401.83
CAS:	82097-50-5

Physical Properties

Property code	Value	Unit	Source
logp	1.317		Crippen Method
mcvol	264.140	ml/mol	McGowan Method
tf	459.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

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_Dataset/1031637
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/110-472-5/Triasulfuron.pdf>

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