

Bromuconazole

Inchi:	InChI=1S/C13H12BrCl2N3O/c14-9-4-13(20-5-9,6-19-8-17-7-18-19)11-2-1-10(15)3-12(11
InchiKey:	HJJVPARKXDDIQD-UHFFFAOYSA-N
Formula:	C13H12BrCl2N3O
SMILES:	Clc1ccc(C2(Cn3cncn3)CC(Br)CO2)c(Cl)c1
Mol. weight [g/mol]:	377.07
CAS:	116255-48-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.51		Cheméo Relay (1.0)
logp	3.664		Crippen Method
mcvol	217.740	ml/mol	McGowan Method
tf	357.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): McGowan Method:	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
Crippen Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0, beta):	

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/100-774-1/Bromuconazole.pdf>

Generated by Cheméo on 2026-10-30 23:12:20.288895607 +0000 UTC m=+25653.215732902.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.