

ethyl

2-[4-[(6-chloro-1,3-benzoxazol-2-yl)oxy]phenoxy]p

Inchi:	InChI=1S/C18H16ClNO5/c1-3-22-17(21)11(2)23-13-5-7-14(8-6-13)24-18-20-15-9-4-12(1)
InchiKey:	PQKBPHSEKWERTG-UHFFFAOYSA-N
Formula:	C18H16ClNO5
SMILES:	CCOC(=O)C(C)Oc1ccc(Oc2nc3ccc(Cl)cc3o2)cc1
Mol. weight [g/mol]:	361.78
CAS:	66441-23-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.17		Cheméo Relay (1.0)
logp	4.604		Crippen Method
mcvol	249.070	ml/mol	McGowan Method
tf	357.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

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_Dataset/1031637
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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<https://www.cheméo.com/cid/106-224-5/ethyl-2-4-6-chloro-1-3-benzoxazol-2-yl-oxy-phenoxy-propanoate.pdf>

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