

2-(propan-2-ylideneamino)oxyethyl 2-[4-(6-chloroquinoxalin-2-yl)oxyphenoxy]propan

Inchi:	InChI=1S/C22H22ClN3O5/c1-14(2)26-29-11-10-28-22(27)15(3)30-17-5-7-18(8-6-17)31-2
InchiKey:	FROBCXTULYFHEJ-UHFFFAOYSA-N
Formula:	C22H22ClN3O5
SMILES:	CC(C)=NOCCOC(=O)C(C)Oc1ccc(Oc2cnc3cc(Cl)ccc3n2)cc1
Mol. weight [g/mol]:	443.89
CAS:	111479-05-1

Physical Properties

Property code	Value	Unit	Source
logp	4.798		Crippen Method
mcvol	316.790	ml/mol	McGowan Method
tf	339.45	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting
Point Dataset (2014, CC0):
McGowan Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

<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

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point

Latest version available from:

<https://www.cheméo.com/cid/103-667-7/2-propan-2-ylideneamino-oxyethyl-2-4-6-chloroquinoxalin-2-yl-oxyphenoxy-p>

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