

Glisoxepide

Inchi:	InChI=1S/C20H27N5O5S/c1-15-14-18(23-30-15)19(26)21-11-10-16-6-8-17(9-7-16)31(28)
InchiKey:	ZKUDBRCEOBOWLF-UHFFFAOYSA-N
Formula:	C20H27N5O5S
SMILES:	<chem>Cc1cc(C(=O)NCCc2ccc(S(=O)(=O)NC(=O)NN3CCCCC3)cc2)no1</chem>
Mol. weight [g/mol]:	449.53
CAS:	25046-79-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Cheméo Relay (1.0)
logp	1.734		Crippen Method
mcvol	325.580	ml/mol	McGowan Method
tf	462.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

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

Cheméo Relay (1.0):

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/107-521-4/Glisojepide.pdf>

Generated by Cheméo on 2026-10-28 02:20:34.40135664 +0000 UTC m=+19077.464258099.

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