

Gliquidone

Inchi:	InChI=1S/C27H33N3O6S/c1-27(2)23-14-11-20(36-3)17-22(23)24(31)30(25(27)32)16-15
InchiKey:	LLJFMFZYVVLQKT-UHFFFAOYSA-N
Formula:	C27H33N3O6S
SMILES:	COc1ccc2c(c1)C(=O)N(CCc1ccc(S(=O)(=O)NC(=O)NC3CCCCC3)cc1)C(=O)C2(C)C
Mol. weight [g/mol]:	527.64
CAS:	33342-05-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.32		Cheméo Relay (1.0)
logp	3.518		Crippen Method
mcvol	390.660	ml/mol	McGowan Method
tf	454.15	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

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/101-117-9/Gliquidone.pdf>

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