

FLAVOXATE

Other names:	2-Piperidinoethyl 3-methyl-4-oxo-2-phenyl-4H-1-benzopyran-8-carboxylate 4H-1-Benzopyran-8-carboxylic acid, 3-methyl-4-oxo-2-phenyl-, 2-(1-piperidinyl)ethyl ester
Inchi:	InChI=1S/C24H25NO4/c1-17-21(26)19-11-8-12-20(23(19)29-22(17)18-9-4-2-5-10-18)24
InchiKey:	SPIUTQOUKAMGCX-UHFFFAOYSA-N
Formula:	C24H25NO4
SMILES:	<chem>Cc1c(-c2ccccc2)oc2c(C(=O)OCCN3CCCCC3)cccc2c1=O</chem>
Mol. weight [g/mol]:	391.47

Physical Properties

Property code	Value	Unit	Source
logp	4.411		Crippen Method
mcvol	300.340	ml/mol	McGowan Method
rinpol	3184.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C15301696&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/58-509-3/FLAVOXATE.pdf>

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