

Dioxaphetyl butyrate

Other names:	4-Morpholinebutanoic acid, «alpha», «alpha»-diphenyl-, ethyl ester 4-Morpholinebutyric acid, «alpha», «alpha»-diphenyl-, ethyl ester Amidalgon Ethyl «alpha», «alpha»-diphenyl-4-morpholinebutyrate Ethyl 4-morpholino-2,2-diphenylbutyrate Spasmoxal Spasmoxale
Inchi:	InChI=1S/C22H27NO3/c1-2-26-21(24)22(19-9-5-3-6-10-19,20-11-7-4-8-12-20)13-14-23-
InchiKey:	LQGIXNQCOXNCRP-UHFFFAOYSA-N
Formula:	C22H27NO3
SMILES:	CCOC(=O)C(CCN1CCOCC1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	353.45
CAS:	467-86-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	3.258		Crippen Method
mcvol	285.750	ml/mol	McGowan Method
rinpol	2491.00		NIST Webbook
rinpol	2491.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C467867&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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