Ethoheptazine

Other names:	1H-Azepine-4-carboxylic acid, hexahydro-1-methyl-4-phenyl-, ethyl ester
	Aethoheptazin
	Ethyl heptazine
	Wy 401
	Zactane
	Azepine-4-carboxylic acid, hexahydro-1-methyl-4-phenyl-, ethyl ester
	4-Carbethoxy-1-methyl-4-phenylazacycloheptane
	4-Carbethoxy-1-methyl-4-phenylhexamethylenimine
	Ethyl hexahydro-1-methyl-4-phenyl-azepine-4-carboxylate
	Hexahydro-1-methyl-4-phenyl-4-azepinecarboxylic acid ethyl ester
	1-Methyl-4-carbethoxy-4-phenylhexamethyleneimine
	1-Methyl-4-carbethoxy-4-phenylhexamethylenimine
	Ethyl hexahydro-1-methyl-4-phenyl-1H-azepine-4-carboxylate
Inchi:	InChI=1S/C16H23NO2/c1-3-19-15(18)16(14-8-5-4-6-9-14)10-7-12-17(2)13-11-16/h4-6,8-
InchiKey:	WGJHHMKQBWSQIY-UHFFFAOYSA-N
Formula:	C16H23NO2
SMILES:	CCOC(=O)C1(c2ccccc2)CCCN(C)CC1
Mol. weight [g/mol]:	261.36
CAS:	77-15-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.62		Crippen Method
logp	2.603		Crippen Method
mcvol	219.100	ml/mol	McGowan Method
rinpol	1840.00		NIST Webbook
rinpol	1848.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1845.00		NIST Webbook
rinpol	1823.00		NIST Webbook
rinpol	1857.00		NIST Webbook
rinpol	1823.00		NIST Webbook
rinpol	1836.00		NIST Webbook
ripol	2453.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C77156&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
ripol:	Polar retention indices