Pyrrocaine

Other names:	1-Pyrrolidineacetamide, N-(2,6-dimethylphenyl)-
	1-Pyrrolidineaceto-2',6'-xylidide
	1-Pyrrolidinoaceto-2',6'-xylidide
	Dynacaine
	EN-1010
	Endocaine
	NSC-52644
Inchi:	InChI=1S/C14H20N2O/c1-11-6-5-7-12(2)14(11)15-13(17)10-16-8-3-4-9-16/h5-7H,3-4,8-1
InchiKey:	OYCGKECKIVYHTN-UHFFFAOYSA-N
Formula:	C14H20N2O
SMILES:	Cc1cccc(C)c1NC(=O)CN1CCCC1
Mol. weight [g/mol]:	232.32
CAS:	2210-77-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.76		Crippen Method
logp	2.338		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
rinpol	1968.00		NIST Webbook
rinpol	1968.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2210777&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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