4,7,13,16,21-Pentaoxa-1,10-diazabicyclo[8.8.5]tric

Other names:	4,7,13,16,21-Pentaoxa-1,10-diazabicyclo[8.8.5.]tricosane
	Kryptofix 221
	4,7,16,21-Pentaoxa-1,10-diazabicyclo[8.8.5.]tricosane
Inchi:	InChI=1S/C16H32N2O5/c1-7-19-8-2-18-5-11-22-15-13-20-9-3-17(1)4-10-21-14-16-23-12
InchiKey:	HDLXPNDSLDLJHF-UHFFFAOYSA-N
Formula:	C16H32N2O5
SMILES:	C1COCCN2CCOCCOCCN(CCO1)CCOCC2
Mol. weight [g/mol]:	332.44
CAS:	31364-42-8

Physical Properties

Property code	Value	Unit	Source
ie	7.40	eV	NIST Webbook
ie	7.70	eV	NIST Webbook
log10ws	1.11		Crippen Method
logp	-0.299		Crippen Method
mcvol	263.890	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31364428&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume