

4,7,13,16,21,24-Hexaoxa-1,10-diazabicyclo[8.8.8]h

Other names:

Kryptofix 222
Cryptand 222
Cryptate 222
Cryptating agent 222
Kriptofix 222
Kryptofix Merck 222
2,2,2-Cryptand
13,16,21,24-Hexaoxa-1,10-diazabicyclo-(8,8,8)-hexacosane
Ligand 222
Crypt-2,2,2
Cryptand C 222
Cryptofix 222
Kryptand 222
NSC 264495

Inchi: InChI=1S/C18H36N2O6/c1-7-21-13-14-24-10-4-20-5-11-25-17-15-22-8-2-19(1)3-9-23-16**InchiKey:** AUFVJZSDSXXFOI-UHFFFAOYSA-N**Formula:** C18H36N2O6**SMILES:** C1COCCN2CCOCCOCCN(CCO1)CCOCCOCC2**Mol. weight [g/mol]:** 376.49**CAS:** 23978-09-8

Physical Properties

Property code	Value	Unit	Source
ie	7.50	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
log10ws	1.19		Crippen Method
logp	-0.283		Crippen Method
mcvol	297.940	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C23978098&Units=SI>**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>**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

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