4,7,13,16,21,24-HEXAOXA-1,10-DIAZABICYCLO[8.

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

Physical Properties

Property code	Value	Unit	Source
af	0.5961		Cheméo Relay (1.0)
gf	-82.32	kJ/mol	Cheméo Relay (1.0, beta)
hf	-997.50	kJ/mol	Cheméo Relay (1.0)
hvap	114.34	kJ/mol	Cheméo Relay (1.0)
ie	7.50	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
log10ws	0.66		Cheméo Relay (1.0)
logp	-0.283		Crippen Method
mcvol	297.940	ml/mol	McGowan Method
pc	1074.43	kPa	Cheméo Relay (1.0, beta)
tb	743.20	K	Cheméo Relay (1.0)
tc	980.72	K	Cheméo Relay (1.0)
tf	421.98	K	Cheméo Relay (1.0)
vc	0.963	m3/kmol	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23978098&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume