

Alpha2,alpha4,alpha6-tri(4-morpholinyl)mesitol

Other names:	Alpha
Inchi:	InChI=1S/C21H33N3O4/c25-21-19(16-23-3-9-27-10-4-23)13-18(15-22-1-7-26-8-2-22)14-
InchiKey:	JGTWRXHFXYTN-UHFFFAOYSA-N
Formula:	C21H33N3O4
SMILES:	Oc1c(CN2CCOCC2)cc(CN2CCOCC2)cc1CN1CCOCC1
Mol. weight [g/mol]:	391.51

Physical Properties

Property code	Value	Unit	Source
logp	0.889		Crippen Method
mcvol	303.830	ml/mol	McGowan Method

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=C5464879&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/84-636-3/Alpha2-alpha4-alpha6-tri-4-morpholinyl-mesitol.pdf>

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