Butalamine

Other names:	1,2-Ethanediamine, N,N-dibutyl-N'-(3-phenyl-1,2,4-oxadiazol-5-yl)- 5-([2-(Dibutylamino)ethyl]amino)-3-phenyl-1,2,4-oxadiazole N,N-Dibutyl-N'-(3-phenyl-1,2,4-oxadiazol-5-yl)-1,2-ethanediamine
Inchi:	InChI=1S/C18H28N4O/c1-3-5-13-22(14-6-4-2)15-12-19-18-20-17(21-23-18)16-10-8-7-9-
InchiKey:	VYWQZAARVNRSTR-UHFFFAOYSA-N
Formula:	C18H28N4O
SMILES:	CCCCN(CCCC)CCNc1nc(-c2ccccc2)no1
Mol. weight [g/mol]:	316.44
CAS:	22131-35-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.69		Crippen Method
logp	4.051		Crippen Method
mcvol	267.050	ml/mol	McGowan Method
rinpol	2457.00		NIST Webbook
rinpol	2450.00		NIST Webbook
rinpol	2490.00		NIST Webbook
rinpol	2450.00		NIST Webbook
rinpol	2490.00		NIST Webbook
rinpol	2457.00		NIST Webbook
rinpol	2450.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22131357&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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