1-Propanamine, N,N-dimethyl-3-[[1-(phenylmethyl)-1H-indazol-3-yl

Other names: 1H-Indazole, 1-benzyl-3-(3-(dimethylamino)propoxy)-
Benzindamine
Benzydamine
1-Benzyl-3-(3-(dimethylamino)propoxy)-1H-indazole

Inchi: InChI=1S/C19H23N3O/c1-21(2)13-8-14-23-19-17-11-6-7-12-18(17)22(20-19)15-16-9-4-3

InchiKey: CNBGNNVCVSKAQZ-UHFFFAOYSA-N

Formula: C19H23N3O

SMILES: CN(C)CCCOc1nn(Cc2ccccc2)c2ccccc12

Mol. weight [g/mol]: 309.41

CAS: 642-72-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.97		Crippen Method
logp	3.415		Crippen Method
mcvol	251.700	ml/mol	McGowan Method
rinpol	2391.00		NIST Webbook
rinpol	2414.00		NIST Webbook
rinpol	2410.00		NIST Webbook
rinpol	2350.00		NIST Webbook
rinpol	2390.00		NIST Webbook
rinpol	2368.00		NIST Webbook
rinpol	2368.00		NIST Webbook
rinpol	2391.00		NIST Webbook
rinpol	2368.00		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=C642728&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

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