

Imidazole-5-sulfonamide,4-(benzylamino)-n,n-dibe

Inchi:	InChI=1S/C24H24N4O2S/c29-31(30,24-23(26-19-27-24)25-16-20-10-4-1-5-11-20)28(17-
InchiKey:	IYUXTOIKTNIVOM-UHFFFAOYSA-N
Formula:	C24H24N4O2S
SMILES:	O=S(=O)(c1[nH]cnc1NCc1ccccc1)N(Cc1ccccc1)Cc1ccccc1
Mol. weight [g/mol]:	432.54
CAS:	116401-57-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.47		Crippen Method
logp	3.931		Crippen Method
mcvol	326.290	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C116401571&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/95-807-1/Imidazole-5-sulfonamide-4-benzylamino-n-n-dibenzyl.pdf>

Generated by Cheméo on 2024-05-17 07:27:39.586009734 +0000 UTC m=+18220108.506587049.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.