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/ci990307l
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