

N-(2-butynyl)-n'-(o-methoxyphenyl)piperazine

Inchi:	InChI=1S/C15H20N2O/c1-3-4-9-16-10-12-17(13-11-16)14-7-5-6-8-15(14)18-2/h5-8H,9-1
InchiKey:	BMWYNORQBVBWPF-UHFFFAOYSA-N
Formula:	C15H20N2O
SMILES:	CC#CCN1CCN(c2ccccc2OC)CC1
Mol. weight [g/mol]:	244.33
CAS:	116594-88-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.27		Crippen Method
logp	1.840		Crippen Method
mcvol	204.820	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=C116594888&Units=SI

Legend

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

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