M-phenylene bis-(2-3-methylpyrazyl) ether

Inchi: InChI=1S/C16H14N4O2/c1-11-15(19-8-6-17-11)21-13-4-3-5-14(10-13)22-16-12(2)18-7-9

InchiKey: DCROVDCZNCUJTR-UHFFFAOYSA-N

Formula: C16H14N4O2

SMILES: Cc1nccnc1Oc1cccc(Oc2nccnc2C)c1

Mol. weight [g/mol]: 294.31

CAS: 116659-49-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	3.468		Crippen Method
mcvol	216.680	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116659495&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume