2-Phenoxy-3-triphenylmethyl pyrazine

Inchi: InChI=1S/C29H22N2O/c1-5-13-23(14-6-1)29(24-15-7-2-8-16-24,25-17-9-3-10-18-25)27-
InchiKey: ZNNRYLHGUSCYJU-UHFFFAOYSA-N
Formula: C29H22N2O
SMILES: c1ccc(Oc2nccnc2C(c2ccccc2)(c2ccccc2)c2ccccc2)cc1
Mol. weight [g/mol]: 414.50
CAS: 116659-47-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.85		Crippen Method
logp	6.652		Crippen Method
mcvol	326.500	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116659473&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