2-Phenoxy-3-methyl pyrazine

Other names:	2-methyl-3-phenoxypyrazine
	Pyrazine, 2-methyl-3-(phenyloxy)
	Pyrazine, 3-methyl-2-phenoxy
	Pyrazine, 2-methyl-3-phenoxy
Inchi:	InChI=1S/C11H10N2O/c1-9-11(13-8-7-12-9)14-10-5-3-2-4-6-10/h2-8H,1H3
InchiKey:	ACDOXXMFLCWEPV-UHFFFAOYSA-N
Formula:	C11H10N2O
SMILES:	Cc1nccnc1Oc1ccccc1
Mol. weight [g/mol]:	186.21
CAS:	91137-78-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	2.577		Crippen Method
mcvol	144.160	ml/mol	McGowan Method
rinpol	1465.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1465.00		NIST Webbook
ripol	2103.00		NIST Webbook
ripol	2103.00		NIST Webbook
ripol	2103.00		NIST Webbook

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=C91137789&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices