2-Phenoxy pyrazine

Other names:	Phenoxypyrazine
	Pyrazine, phenoxy-
Inchi:	InChI=1S/C10H8N2O/c1-2-4-9(5-3-1)13-10-8-11-6-7-12-10/h1-8H
InchiKey:	LKXUZLSVURTETC-UHFFFAOYSA-N
Formula:	C10H8N2O
SMILES:	c1ccc(Oc2cnccn2)cc1
Mol. weight [g/mol]:	172.18
CAS:	107697-82-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Crippen Method
logp	2.269		Crippen Method
mcvol	130.070	ml/mol	McGowan Method
rinpol	1415.00		NIST Webbook
rinpol	1415.00		NIST Webbook
ripol	2104.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107697825&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
rinpol:	Non-polar retention indices

ripol: Polar retention indices

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