2-isopropyl-3-ethoxypyrazine

Other names:	3-isopropyl-2-ethoxypyrazine
	2-Ethoxy-3-isopropylpyrazine
	Pyrazine, 2-ethoxy-3-(1-methylethyl)-
Inchi:	InChI=1S/C9H14N2O/c1-4-12-9-8(7(2)3)10-5-6-11-9/h5-7H,4H2,1-3H3
InchiKey:	LTAUBPVQMBOANV-UHFFFAOYSA-N
Formula:	C9H14N2O
SMILES:	CCOc1nccnc1C(C)C
Mol. weight [g/mol]:	166.22
CAS:	72797-16-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	1.999		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
rinpol	1143.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1143.00		NIST Webbook
ripol	1431.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72797161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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