Pyrazine, (2-phenylethyl)-

Other names:	Pyrazine, phenethyl- (2-Phenylethyl)pyrazine Phenylethyl-pyrazine
Inchi:	InChI=1S/C12H12N2/c1-2-4-11(5-3-1)6-7-12-10-13-8-9-14-12/h1-5,8-10H,6-7H2
InchiKey:	LQWPAMNCTNMMDB-UHFFFAOYSA-N
Formula:	C12H12N2
SMILES:	c1ccc(CCc2cnccn2)cc1
Mol. weight [g/mol]:	184.24
CAS:	91391-83-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	2.262		Crippen Method
mcvol	152.380	ml/mol	McGowan Method
rinpol	1552.00		NIST Webbook
ripol	2367.00		NIST Webbook
ripol	2351.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91391832&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