n-Pentylpyrazine

Other names:	n-Amylpyrazine
	Pyrazine, pentyl-
	2-Pentylpyrazine
	Pentyl pyrazine
Inchi:	InChI=1S/C9H14N2/c1-2-3-4-5-9-8-10-6-7-11-9/h6-8H,2-5H2,1H3
InchiKey:	KNDDHUQSPNJCKY-UHFFFAOYSA-N
Formula:	C9H14N2
SMILES:	CCCCCc1cnccn1
Mol. weight [g/mol]:	150.22
CAS:	6303-75-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	2.209		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1192.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1192.00		NIST Webbook
ripol	1575.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6303759&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