triethylmethylpyrazine

Inchi:	InChI=1S/C11H18N2/c1-5-9-8(4)12-10(6-2)11(7-3)13-9/h5-7H2,1-4H3
InchiKey:	ICSINJKWHMSKAK-UHFFFAOYSA-N
Formula:	C11H18N2
SMILES:	CCc1nc(CC)c(CC)nc1C
Mol. weight [g/mol]:	178.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.89		Crippen Method
logp	2.472		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
ripol	1560.00		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=R297037&Units=SI

Legend

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

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