2,3,5-Trimethyl-6-propylpyrazine

Other names:	2-Propyl-3,5,6-trimethylpyrazine
	Trimethylpropylpyrazine
Inchi:	InChI=1S/C10H16N2/c1-5-6-10-9(4)11-7(2)8(3)12-10/h5-6H2,1-4H3
InchiKey:	GEPYSCIASYXPCY-UHFFFAOYSA-N
Formula:	C10H16N2
SMILES:	CCCc1nc(C)c(C)nc1C
Mol. weight [g/mol]:	164.25
CAS:	92233-82-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.65		Crippen Method
logp	2.354		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
rinpol	1280.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1233.00		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=C92233824&Units=SI

Legend

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

rinpol: Non-polar retention indices

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