2-Methyl-3-propylpyrazine

Other names:	3-Propyl-2-methyl pyrazine
	2-Methyl-3-n-propylpyrazine
	2-Propyl-3-methylpyrazine
	Pyrazine, 2-methyl-3-propyl-
Inchi:	InChI=1S/C8H12N2/c1-3-4-8-7(2)9-5-6-10-8/h5-6H,3-4H2,1-2H3
InchiKey:	XAWKNALRUSOTOY-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	CCCc1nccnc1C
Mol. weight [g/mol]:	136.19
CAS:	15986-80-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	1.738		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
rinpol	1088.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1065.00		NIST Webbook
ripol	1461.00		NIST Webbook
ripol	1479.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1489.00		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1462.00		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1461.00		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=C15986808&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
ripol:	Polar retention indices