Pyrazine, 5-butyl-2,3-dimethyl-

Other names:	5-Butyl-2,3-dimethylpyrazine
	2,3-Dimethyl-5-butylpyrazine
Inchi:	InChI=1S/C10H16N2/c1-4-5-6-10-7-11-8(2)9(3)12-10/h7H,4-6H2,1-3H3
InchiKey:	RYKQVGCVJZOAAN-UHFFFAOYSA-N
Formula:	C10H16N2
SMILES:	CCCCc1cnc(C)c(C)n1
Mol. weight [g/mol]:	164.25
CAS:	15834-78-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.436		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
rinpol	1198.00		NIST Webbook
rinpol	1254.00		NIST Webbook
ripol	1600.00		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=C15834783&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