Pyrazine, 6-ethyl-3-methyl-2-(2-methylpropyl)

Other names:	3-methyl-6-ethyl-2-isobutylpyrazine
Inchi:	InChI=1S/C11H18N2/c1-5-10-7-12-9(4)11(13-10)6-8(2)3/h7-8H,5-6H2,1-4H3
InchiKey:	IWDMYXZBSTZHFS-UHFFFAOYSA-N
Formula:	C11H18N2
SMILES:	CCc1cnc(C)c(CC(C)C)n1
Mol. weight [g/mol]:	178.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Crippen Method
logp	2.546		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
ripol	1580.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R266409&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:
https://www.chemeo.com/cid/78-866-5/Pyrazine-6-ethyl-3-methyl-2-2-methylpropyl.pdf
Generated by Cheméo on 2024-10-12 04:05:15.031406044 +0000 UTC m=+3286777.668375292.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.