

2-METHYLTHIO-3-ETHYLPYRAZINE

Other names:	2-(Methylthio)-3-ethylpyrazine 2-Ethyl-3-methylthiopyrazine 3-Ethyl-2-(methylthio)pyrazine Pyrazine, 3-ethyl-2-(methylthio)
Inchi:	InChI=1S/C7H10N2S/c1-3-6-7(10-2)9-5-4-8-6/h4-5H,3H2,1-2H3
InchiKey:	XYHPPOMSLGJAAM-UHFFFAOYSA-N
Formula:	C7H10N2S
SMILES:	CCc1nccnc1SC
Mol. weight [g/mol]:	154.24

Physical Properties

Property code	Value	Unit	Source
ie	8.38	eV	Cheméo Relay (1.0)
logp	1.761		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
tb	501.88	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72987623&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

tb: Normal Boiling Point Temperature

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