

2-ETHOXY-3-ETHYLPYRAZINE

Other names:	3-Ethyl-2-ethoxypyrazine Pyrazine, 2-ethoxy-3-ethyl Pyrazine, 3-ethoxy-2-ethyl
Inchi:	InChI=1S/C8H12N2O/c1-3-7-8(11-4-2)10-6-5-9-7/h5-6H,3-4H2,1-2H3
InchiKey:	TYSHGGVMHVIOMH-UHFFFAOYSA-N
Formula:	C8H12N2O
SMILES:	CCOc1nccnc1CC
Mol. weight [g/mol]:	152.20

Physical Properties

Property code	Value	Unit	Source
logp	1.438		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
rinpol	1101.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1101.00		NIST Webbook
rinpol	1101.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1101.00		NIST Webbook
ripol	1439.00		NIST Webbook
ripol	1439.00		NIST Webbook
ripol	1439.00		NIST Webbook
ripol	1439.00		NIST Webbook
tb	468.24	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35243437&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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