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]:	152.19
CAS:	35243-43-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Crippen Method
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	1127.00		NIST Webbook
rinpol	1101.00		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

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=C35243437&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

Latest version available from:
https://www.chemeo.com/cid/25-611-5/2-Ethoxy-3-ethylpyrazine.pdf
Generated by Cheméo on 2024-04-26 10:13:06.691155961 +0000 UTC m=+16415635.611733277.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.