2-Ethyl-3-methoxypyrazine

Other names:	2-Methoxy-3-ethylpyrazine
	Pyrazine, 2-ethyl-3-methoxy-
	3-Ethyl-2-methoxypyrazine
	Pyrazine, 3-ethyl-2-methoxy
Inchi:	InChI=1S/C7H10N2O/c1-3-6-7(10-2)9-5-4-8-6/h4-5H,3H2,1-2H3
InchiKey:	DPCILIMHENXHQX-UHFFFAOYSA-N
Formula:	C7H10N2O
SMILES:	CCc1nccnc1OC
Mol. weight [g/mol]:	138.17
CAS:	25680-58-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.93		Crippen Method
logp	1.048		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
rinpol	1037.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1063.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1400.00		NIST Webbook

Sources

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=C25680584&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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