

Pyrazine, methoxy-

Other names:	2-Methoxypyrazine methoxypyrazine
Inchi:	InChI=1S/C5H6N2O/c1-8-5-4-6-2-3-7-5/h2-4H,1H3
InchiKey:	WKSXRWSOSLGSTN-UHFFFAOYSA-N
Formula:	C5H6N2O
SMILES:	COc1cnccn1
Mol. weight [g/mol]:	110.11
CAS:	3149-28-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.12		Crippen Method
logp	0.485		Crippen Method
mcvol	83.380	ml/mol	McGowan Method
rinpol	877.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	896.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	904.00		NIST Webbook
ripol	1306.00		NIST Webbook
ripol	1306.00		NIST Webbook
ripol	1306.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	334.20	K	3.90	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3149288&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Pyrazine and Its Derivatives in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je0601457

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
tbrp:	Boiling point at reduced pressure

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