

1-Piperazinecarboxaldehyde

Other names:	1-Formylpiperazine N-Formylpiperazine Formylpiperazine piperazine-1-carbaldehyde
Inchi:	InChI=1S/C5H10N2O/c8-5-7-3-1-6-2-4-7/h5-6H,1-4H2
InchiKey:	MSSDTZLYNMFTKN-UHFFFAOYSA-N
Formula:	C5H10N2O
SMILES:	O=CN1CCNCC1
Mol. weight [g/mol]:	114.15
CAS:	7755-92-2

Physical Properties

Property code	Value	Unit	Source
log10ws	0.66		Crippen Method
logp	-0.952		Crippen Method
mcvol	91.980	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.70	K	0.07	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7755922&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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