1H-Pyrrole-2-carboxaldehyde, 1-methyl-

Other names:	2-Formyl-1-methylpyrrole
	N-Methyl-2-formylpyrrole
	1-Methyl-2-formylpyrrole
	N-Methylpyrrole-2-carboxaldehyde
	1-Methyl-1H-pyrrole-2-carboxaldehyde
	1-Methylpyrrole-2-carboxaldehyde
	Pyrrole-2-carboxaldehyde, 1-methyl-
	N-Methylpyrrole-2-carbaldehyde
	1-Methyl-1H-pyrrole-2-carbaldehyde
	1-Methyl-2-pyrrolaldehyde
	1-Methyl-2-pyrrolecarboxaldehyde
	1-Methylpyrrole-2-carbaldehyde
	1-Methylpyrrole-2-carboxyaldehyde
	N-Methylpyrrole-2-carboxy aldehyde
	NSC 72386
	1-methylformylpyrrole
Inchi:	InChI=1S/C6H7NO/c1-7-4-2-3-6(7)5-8/h2-5H,1H3
InchiKey:	OUKQTRFCDKSEPL-UHFFFAOYSA-N
Formula:	C6H7NO
SMILES:	Cn1cccc1C=O
Mol. weight [g/mol]:	109.13
CAS:	1192-58-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.00		Crippen Method
logp	0.838		Crippen Method
mcvol	87.490	ml/mol	McGowan Method
rinpol	1010.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	1010.00		NIST Webbook

rinpol	1015.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	986.00	NIST Webbook
rinpol	975.00	NIST Webbook
rinpol	1022.00	NIST Webbook
rinpol	1010.00	NIST Webbook
ripol	1610.00	NIST Webbook
ripol	1626.00	NIST Webbook
ripol	1637.00	NIST Webbook
ripol	1620.00	NIST Webbook
ripol	1620.00	NIST Webbook
ripol	1618.00	NIST Webbook
ripol	1606.00	NIST Webbook
ripol	1615.00	NIST Webbook
ripol	1651.00	NIST Webbook
ripol	1632.00	NIST Webbook
ripol	1661.00	NIST Webbook
ripol	1661.00	NIST Webbook
ripol	1661.00	NIST Webbook
ripol	1583.00	NIST Webbook
ripol	1626.00	NIST Webbook
ripol	1632.00	NIST Webbook
ripol	1607.00	NIST Webbook
ripol	1661.00	NIST Webbook
ripol	1616.00	NIST Webbook
ripol	1637.00	NIST Webbook
ripol	1606.00	NIST Webbook
ripol	1661.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.70	K	2.90	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1192581&Units=SI

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

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