1-(Fur-2-ylmethyl)-2-formyl-pyrrole

Other names:	1-furfuryl-2-formylpyrrole
	1-(2-furanylmethyl)-2-formyl- 1H-pyrrole
	1-(2-furfuryl)pyrrole-2-carboxaldehyde
	Pyrrole-2-carboxaldehyde, 1-(2-furfuryl)
Inchi:	InChI=1S/C10H9NO2/c12-8-9-3-1-5-11(9)7-10-4-2-6-13-10/h1-6,8H,7H2
InchiKey:	PYBJPTHZYBWJON-UHFFFAOYSA-N
Formula:	C10H9NO2
SMILES:	O=Cc1cccn1Cc1ccco1
Mol. weight [g/mol]:	175.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.01		Crippen Method
logp	1.942		Crippen Method
mcvol	130.260	ml/mol	McGowan Method
rinpol	1374.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1384.00		NIST Webbook
ripol	2254.00		NIST Webbook
ripol	2266.00		NIST Webbook
ripol	2266.00		NIST Webbook
ripol	2254.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R87946&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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