2-Propionylpyrrole

Other names:	1H-Pyrrole, 2-propionyl
	Pyrrole, 2-propionyl
	1-(1H-pyrrol-2-yl)propan-1-one
Inchi:	InChI=1S/C7H9NO/c1-2-7(9)6-4-3-5-8-6/h3-5,8H,2H2,1H3
InchiKey:	AEJPPSRYXGEVDT-UHFFFAOYSA-N
Formula:	C7H9NO
SMILES:	CCC(=O)c1ccc[nH]1
Mol. weight [g/mol]:	123.15
CAS:	1073-26-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.77		Crippen Method
logp	1.125		Crippen Method
mcvol	101.580	ml/mol	McGowan Method
rinpol	1026.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1026.00		NIST Webbook
ripol	1990.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1073263&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

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