2-(2-Furyl)-5(6)-acetylpyrazine

Inchi: InChI=1S/C10H8N2O2/c1-7(13)8-5-12-9(6-11-8)10-3-2-4-14-10/h2-6H,1H3
InchiKey: NZQVQHPEBQZZFF-UHFFFAOYSA-N
Formula: C10H8N2O2
SMILES: CC(=O)c1cnc(-c2ccco2)cn1
Mol. weight [g/mol]: 188.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.00		Crippen Method
logp	1.939		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
rinpol	1573.00		NIST Webbook
rinpol	1573.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R87964&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.