3-ACETAMIDOFURAN

Inchi: InChI=1S/C6H7NO2/c1-5(8)7-6-2-3-9-4-6/h2-4H,1H3,(H,7,8)
InchiKey: MSUYGSATOVDCFI-UHFFFAOYSA-N
Formula: C6H7NO2
SMILES: CC(=O)Nc1ccoc1
Mol. weight [g/mol]: 125.13

Physical Properties

Property code	Value	Unit	Source
ie	8.57	eV	Cheméo Relay (1.0)
log10ws	-0.75		Cheméo Relay (1.0)
logp	1.238		Crippen Method
mcvol	93.360	ml/mol	McGowan Method
rinpol	1202.00		NIST Webbook
rinpol	1202.00		NIST Webbook
tb	503.30	K	Cheméo Relay (1.0)
tf	334.75	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C59445851&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point