1-Acetyl-4-methylpiperazine

Inchi: InChI=1S/C7H14N2O/c1-7(10)9-5-3-8(2)4-6-9/h3-6H2,1-2H3
InchiKey: YSDBJKNOEWSFGA-UHFFFAOYSA-N
Formula: C7H14N2O
SMILES: CC(=O)N1CCN(C)CC1
Mol. weight [g/mol]: 142.20
CAS: 60787-05-5

Physical Properties

Property code	Value	Unit	Source
log10ws	0.44		Crippen Method
logp	-0.220		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
rinpol	1288.00		NIST Webbook
rinpol	1288.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C60787055&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