Piperazine, 1,4-diacetyl-

Other names: Benzylpiperazine-M (piperazine), 2AC
Inchi: InChI=1S/C8H14N2O2/c1-7(11)9-3-5-10(6-4-9)8(2)12/h3-6H2,1-2H3
InchiKey: NBQBICYRKOTWRR-UHFFFAOYSA-N
Formula: C8H14N2O2
SMILES: CC(=O)N1CCN(C(C)=O)CC1
Mol. weight [g/mol]: 170.21
CAS: 18940-57-3

Physical Properties

Property code	Value	Unit	Source
log10ws	0.24		Crippen Method
logp	-0.303		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
rinpol	1780.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1750.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18940573&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