3-Piperidinol, 1-acetyl-6-propyl-, (3R-trans)-

Inchi: InChI=1S/C10H19NO2/c1-3-4-9-5-6-10(13)7-11(9)8(2)12/h9-10,13H,3-7H2,1-2H3/t9-,10-
InchiKey: MMZIMNFISYOWRF-NXEZZACHSA-N
Formula: C10H19NO2
SMILES: CCCC1CCC(O)CN1C(C)=O
Mol. weight [g/mol]: 185.26
CAS: 54751-92-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.74		Crippen Method
logp	1.158		Crippen Method
mcvol	158.320	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54751927&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume