

Acetamide, 9h-(adenin-9-yl)-

Inchi: InChI=1S/C7H8N6O/c8-4(14)1-13-3-12-5-6(9)10-2-11-7(5)13/h2-3H,1H2,(H2,8,14)(H2,9,
InchiKey: RVZMUNXBWYWNJA-UHFFFAOYSA-N
Formula: C7H8N6O
SMILES: NC(=O)Cn1cnc2c(N)ncnc21
Mol. weight [g/mol]: 192.18
CAS: 98277-56-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.68		Crippen Method
logp	-1.106		Crippen Method
mcvol	132.020	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C98277566&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

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<https://www.chemeo.com/cid/62-387-4/Acetamide-9h-adenin-9-yl.pdf>

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