9H-imidazo[2,1-i]purine, 9-ethyl-7,8-dihydro-

Inchi: InChI=1S/C9H11N5/c1-2-13-3-4-14-6-12-8-7(9(13)14)10-5-11-8/h5-6H,2-4H2,1H3
InchiKey: XEZIACMXBMYRPT-UHFFFAOYSA-N
Formula: C9H11N5
SMILES: CCN1CCn2cnc3ncnc-3c21
Mol. weight [g/mol]: 189.22
CAS: 93227-13-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.85		Crippen Method
logp	0.618		Crippen Method
mcvol	137.790	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=C93227135&Units=SI

Legend

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