6-ethoxy-9H-purine

Other names: 6-ethoxy-1H-purine
Inchi: InChI=1S/C7H8N4O/c1-2-12-7-5-6(9-3-8-5)10-4-11-7/h3-4H,2H2,1H3,(H,8,9,10,11)
InchiKey: BMLKPGJBYUTIHT-UHFFFAOYSA-N
Formula: C7H8N4O
SMILES: CCOc1ncnc2nc[nH]c12
Mol. weight [g/mol]: 164.17

Physical Properties

Property code	Value	Unit	Source
logp	0.270		Crippen Method
mcvol	116.360	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17861062&Units=SI

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:
https://www.chemeo.com/cid/65-117-0/6-ethoxy-9H-purine.pdf
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