Allopurinol di-methyl derivative

Other names: Allopurinol, dimethyl
Inchi: InChI=1S/C7H8N4O/c1-10-4-8-6-5(7(10)12)3-9-11(6)2/h3-4H,1-2H3
InchiKey: PVQKQWMEXZGTMR-UHFFFAOYSA-N
Formula: C7H8N4O
SMILES: Cn1cnc2c(cnn2C)c1=O
Mol. weight [g/mol]: 164.16
CAS: 5334-54-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.81		Crippen Method
logp	-0.333		Crippen Method
mcvol	116.360	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5334543&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