

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:	<chem>Cn1cnc2c(cnn2C)c1=O</chem>
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

Latest version available from:

<https://www.chemeo.com/cid/29-112-5/Allopurinol-di-methyl-derivative.pdf>

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