

7H-imidazo[4,5-d]-v-triazin-4-ol, 7-butyl-, (keto form)

Inchi:	InChI=1S/C8H11N5O/c1-2-3-4-13-5-9-6-7(13)10-12-11-8(6)14/h5H,2-4H2,1H3,(H,10,11,
InchiKey:	QYQAOLAKBZEERN-UHFFFAOYSA-N
Formula:	C8H11N5O
SMILES:	CCCCn1cnc2c(=O)[nH]nnc21
Mol. weight [g/mol]:	193.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	-0.167		Crippen Method
mcvol	140.430	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=B6008701&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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