

V-triazolo[5,4-d]-v-triazin-7(6h)-one

Inchi:	InChI=1S/C3H2N6O/c10-3-1-2(5-8-4-1)6-9-7-3/h(H2,4,5,6,7,8,10)
InchiKey:	VKEOBKIFUVFEHF-UHFFFAOYSA-N
Formula:	C3H2N6O
SMILES:	O=c1[nH]nnc2[nH]nnc12
Mol. weight [g/mol]:	138.09
CAS:	4730-53-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.20		Crippen Method
logp	-2.528		Crippen Method
mcvol	79.960	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C4730534&Units=SI

Legend

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

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