

Pyrazolo[1,5-d][1,2,4]triazin-3-one, 2,5,6-trimethyl-7,7-pentamethylene

Inchi:	InChI=1S/C13H20N4O/c1-10-12(18)11-9-15(2)16(3)13(17(11)14-10)7-5-4-6-8-13/h9H,4-
InchiKey:	SYTRPDHLDZPMR-UHFFFAOYSA-N
Formula:	C13H20N4O
SMILES:	CC1=NN2C(=CN(C)N(C)C23CCCCC3)C1=O
Mol. weight [g/mol]:	248.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	1.541		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
rinpola	1939.00		NIST Webbook

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=R154633&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvola:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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