

4,5,6,7-Tetrahydropyrazolo[1,5-d][1,2,4]-triazin-4-one-2,5-dimethyl-7,7-tetramethylene

InChI: Cc1nc2c(c1)nc(=O)n2C(C)C(C)C(C)C(C)C
InChIKey: UURHHYSBRAMJBX-UHFFFAOYSA-N
Formula: C₁₁H₁₈N₄O
SMILES: CC1=NN2C(C1)C(=O)N(C)NC21CCCC1
Mol. weight [g/mol]: 222.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.08		Crippen Method
logp	0.684		Crippen Method
mcvol	170.460	ml/mol	McGowan Method
rinpol	1842.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=R582320&Units=SI>

Legend

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

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