

7-(1,3-dioxolan-2-ylmethyl)-1,3-dimethylpurine-2,6

Inchi:	InChI=1S/C11H14N4O4/c1-13-9-8(10(16)14(2)11(13)17)15(6-12-9)5-7-18-3-4-19-7/h6-7
InchiKey:	HWXIGFIVGWUZAQ-UHFFFAOYSA-N
Formula:	C11H14N4O4
SMILES:	Cn1c(=O)c2c(ncn2CC2OCCO2)n(C)c1=O
Mol. weight [g/mol]:	266.26
CAS:	69975-86-6

Physical Properties

Property code	Value	Unit	Source
ie	8.19	eV	Cheméo Relay (1.0)
log10ws	-0.57		Cheméo Relay (1.0)
logp	-1.193		Crippen Method
mcvol	179.470	ml/mol	McGowan Method
tf	417.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):
McGowan Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

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

tf: Normal melting (fusion) point

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