[1-(dimethylcarbamoyl)-5-methylpyrazol-3-yl] N,N-dimethylcarbamate

Inchi: InChI=1S/C10H16N4O3/c1-7-6-8(17-10(16)13(4)5)11-14(7)9(15)12(2)3/h6H,1-5H3

InchiKey: RDBIYWSVMRVKSG-UHFFFAOYSA-N

Formula: C10H16N4O3

SMILES: Cc1cc(OC(=O)N(C)C)nn1C(=O)N(C)C

Mol. weight [g/mol]: 240.26

CAS: 644-64-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.32		Cheméo Relay (1.0)
logp	0.782		Crippen Method
mcvol	181.230	ml/mol	McGowan Method
tf	342.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637

McGowan Method: 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):

Cheméo Relay (1.0, beta):

Legend

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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