Carmofur

Inchi: InChI=1S/C11H16FN3O3/c1-2-3-4-5-6-13-10(17)15-7-8(12)9(16)14-11(15)18/h7H,2-6H2
InchiKey: AOCCBINRVIKJHY-UHFFFAOYSA-N
Formula: C11H16FN3O3
SMILES: CCCCCCNC(=O)n1cc(F)c(=O)[nH]c1=O
Mol. weight [g/mol]: 257.27
CAS: 61422-45-5

Physical Properties

Property code	Value	Unit	Source
logp	0.332		Crippen Method
mcvol	187.110	ml/mol	McGowan Method
tf	383.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

Latest version available from:

https://www.chemeo.com/cid/110-948-7/Carmofur.pdf

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