

Creatinine, N,N'-di(pentafluoropropionyl)-

Inchi: InChI=1S/C10H5F10N3O3/c1-22-2-3(24)23(5(26)8(13,14)10(18,19)20)6(22)21-4(25)7(1
InchiKey: QEPIGSHFFFKQNB-UHFFFAOYSA-N
Formula: C10H5F10N3O3
SMILES: CN1CC(=O)N(C(=O)C(F)(F)C(F)(F)F)C1=NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 405.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Crippen Method
logp	1.565		Crippen Method
mcvol	188.950	ml/mol	McGowan Method
rinpol	1889.00		NIST Webbook
rinpol	1889.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U374352&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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<https://www.cheméo.com/cid/61-915-8/Creatinine-N-N-di-pentafluoropropionyl.pdf>

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