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(11
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/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=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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