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

Inchi: InChI=1S/C12H5F14N3O3/c1-28-2-3(30)29(5(32)8(15,16)10(19,20)12(24,25)26)6(28)27-
InchiKey: BLGWIZSZDSJYCV-UHFFFAOYSA-N
Formula: C12H5F14N3O3
SMILES: CN1CC(=O)N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)C1=NC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 505.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.94		Crippen Method
logp	2.835		Crippen Method
mcvol	224.210	ml/mol	McGowan Method
rinpol	1982.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374353&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices