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

Inchi: InChI=1S/C12H3F14N3O3/c13-7(14,9(17,18)11(21,22)23)4(30)27-3-1-2-29(6(32)28-3)5(
InchiKey: OJZTTZGAXKFHHU-UHFFFAOYSA-N
Formula: C12H3F14N3O3
SMILES: O=C(Nc1ccn(C(=O)C(F)(F)C(F)(F)C(F)(F)F)c(=O)n1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 503.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.24		Crippen Method
logp	3.488		Crippen Method
mcvol	219.910	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374746&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume