

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(31)6
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.cheméo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/79-447-9/Cytosine-N-N-di-heptafluorobutyryl.pdf>

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