Adenine, N4-heptafluorobutyryl-

Inchi: InChI=1S/C9H4F7N5O/c10-7(11,8(12,13)9(14,15)16)6(22)21-5-3-4(18-1-17-3)19-2-20-5/
InchiKey: SPFZCSCQDNMESQ-UHFFFAOYSA-N
Formula: C9H4F7N5O
SMILES: O=C(Nc1ncnc2[nH]cnc12)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 331.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.12		Crippen Method
logp	1.642		Crippen Method
mcvol	162.610	ml/mol	McGowan Method
rinpol	1766.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374883&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
rinpol: Non-polar retention indices