N-Nitrosodimethylamine, HFBA-derivative

Inchi: InChI=1S/C12H8F14N4O3/c13-7(14,9(17,18)11(21,22)23)5(31)30(29-3-1-28(27-33)2-4-2
InchiKey: CQGSIHUFUNTCMI-UHFFFAOYSA-N
Formula: C12H8F14N4O3
SMILES: O=NN1CCN(N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)C(F)(F)F)CC1
Mol. weight [g/mol]: 522.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	3.221		Crippen Method
mcvol	238.490	ml/mol	McGowan Method
rinpol	1335.00		NIST Webbook
rinpol	1335.00		NIST Webbook

Sources

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=R579923&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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