N-tert-Butyl-N-trifluoroacetyl-N'-trifluoroacetyl-N'-

Other names: N-Cyclopropyl-N-trifluoroacetyl-N'-(2-methyl-2-propanyl)-N'-trifluoroacetyl-6-(methylsulfan
Inchi: InChI=1S/C15H17F6N5O2S/c1-13(2,3)26(9(28)15(19,20)21)11-22-10(23-12(24-11)29-4)
InchiKey: CJQRQPSSRYVENY-UHFFFAOYSA-N
Formula: C15H17F6N5O2S
SMILES: CSc1nc(N(C(=O)C(F)(F)F)C2CC2)nc(N(C(=O)C(F)(F)F)C(C)(C)C)n1
Mol. weight [g/mol]: 445.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	3.345		Crippen Method
mcvol	267.600	ml/mol	McGowan Method
rinpol	1882.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373107&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.