arginine, trifluoroacetyl-isopropyl ester

Inchi: InChI=1S/C15H17F9N4O5/c1-6(2)33-8(29)7(26-9(30)13(16,17)18)4-3-5-28(11(32)15(22,
InchiKey: KZUWKZBYIITTDX-UHFFFAOYSA-N
Formula: C15H17F9N4O5
SMILES: CC(C)OC(=O)C(CCCN(C(=N)N=C(O)C(F)(F)F)C(=O)C(F)(F)F)N=C(O)C(F)(F)F
Mol. weight [g/mol]: 504.30

Physical Properties

Property code	Value	Unit	Source
hf	-2405.85	kJ/mol	Joback Method
hvap	107.14	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	3.450		Crippen Method
mcvol	285.910	ml/mol	McGowan Method
rinpol	1832.00		NIST Webbook
tb	1089.88	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R267833&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature