

# 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/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/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

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