2-Adamantylamine, N-pentafluoropropionyl-

Inchi: InChI=1S/C13H16F5NO/c14-12(15,13(16,17)18)11(20)19-10-8-2-6-1-7(4-8)5-9(10)3-6/h6
InchiKey: XQQFDPHMUKCPLG-UHFFFAOYSA-N
Formula: C13H16F5NO
SMILES: OC(=NC1C2CC3CC(C2)CC1C3)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 297.26

Physical Properties

Property code	Value	Unit	Source
hf	-1217.94	kJ/mol	Joback Method
hvap	57.22	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.965		Crippen Method
mcvol	181.850	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	1492.00		NIST Webbook
rinpol	1492.00		NIST Webbook
tb	670.62	K	Joback Method
tc	859.54	K	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374751&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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