2-Amino-1-phenylethanol, N,O-bis(pentafluoropropionyl)-

Inchi: InChI=1S/C14H9F10NO3/c15-11(16,13(19,20)21)9(26)25-6-8(7-4-2-1-3-5-7)28-10(27)12

InchiKey: DDVCYTVJYOONKV-UHFFFAOYSA-N

Formula: C14H9F10NO3

SMILES: O=C(OC(CN=C(O)C(F)(F)C(F)(F)F)c1ccccc1)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 429.21

Physical Properties

Property code	Value	Unit	Source
hf	-2421.74	kJ/mol	Joback Method
hvap	64.52	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.623		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	1329.00		NIST Webbook
tb	770.77	K	Joback Method
tc	952.67	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=U376225&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