5-Amino-2-methoxyphenol, O,N-bis(pentafluoropropionyl)-

Inchi: InChI=1S/C13H7F10NO4/c1-27-6-3-2-5(24-8(25)10(14,15)12(18,19)20)4-7(6)28-9(26)11

InchiKey: NLAFAKCFLVJABJ-UHFFFAOYSA-N

Formula: C13H7F10NO4

SMILES: COc1ccc(N=C(O)C(F)(F)C(F)(F)F)cc1OC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 431.18

Physical Properties

Property code	Value	Unit	Source
hf	-2550.98	kJ/mol	Joback Method
hvap	66.42	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.584		Crippen Method
mcvol	212.830	ml/mol	McGowan Method
pc	1577.21	kPa	Joback Method
rinpol	1468.00		NIST Webbook
rinpol	1468.00		NIST Webbook
tb	780.71	K	Joback Method
tc	963.39	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=U374258&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