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

Inchi: InChI=1S/C11H7F6NO4/c1-21-6-3-2-5(18-8(19)10(12,13)14)4-7(6)22-9(20)11(15,16)17/h

InchiKey: NIBNJRKHLJRJMO-UHFFFAOYSA-N

Formula: C11H7F6NO4

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

Mol. weight [g/mol]: 331.17

Physical Properties

Property code	Value	Unit	Source
hf	-1707.76	kJ/mol	Joback Method
hvap	67.83	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.313		Crippen Method
mcvol	177.570	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1481.00		NIST Webbook
tb	744.33	K	Joback Method
tc	933.02	K	Joback Method

Sources

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=U374874&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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