3-Methoxytyramine, di-TFA

Other names: 3-Methoxytyramine, TFA
Inchi: InChI=1S/C13H11F6NO4/c1-23-9-6-7(4-5-20-10(21)12(14,15)16)2-3-8(9)24-11(22)13(17
InchiKey: BCNUYVIWUMREID-UHFFFAOYSA-N
Formula: C13H11F6NO4
SMILES: COc1cc(CCN=C(O)C(F)(F)F)ccc1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 359.22

Physical Properties

Property code	Value	Unit	Source
hf	-1749.04	kJ/mol	Joback Method
hvap	72.28	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.224		Crippen Method
mcvol	205.750	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	1595.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1595.00		NIST Webbook
tb	790.09	K	Joback Method
tc	979.33	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U71885&Units=SI

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