Hippuric acid, TFA-ME

Inchi: InChI=1S/C12H10F3NO4/c1-19-9(17)7-16-10(8-5-3-2-4-6-8)20-11(18)12(13,14)15/h2-6H

InchiKey: IIEUKBPPYQDCCR-UHFFFAOYSA-N

Formula: C12H10F3NO4

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

Mol. weight [g/mol]: 289.21

Physical Properties

Property code	Value	Unit	Source
hf	-1068.73	kJ/mol	Joback Method
hvap	62.54	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.712		Crippen Method
mcvol	182.050	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1530.00		NIST Webbook
tb	724.36	K	Joback Method
tc	936.12	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=R387170&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