propionyl glycine, PFP-TFE

Inchi: InChI=1S/C10H9F8NO4/c1-2-5(19-3-6(20)22-4-8(11,12)13)23-7(21)9(14,15)10(16,17)18
InchiKey: XWRAVIVXSXJGKD-UHFFFAOYSA-N
Formula: C10H9F8NO4
SMILES: CCC(=NCC(=O)OCC(F)(F)F)OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 359.17

Physical Properties

Property code	Value	Unit	Source
hf	-2262.03	kJ/mol	Joback Method
hvap	49.14	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.641		Crippen Method
mcvol	186.480	ml/mol	McGowan Method
pc	1614.17	kPa	Joback Method
rinpol	1073.00		NIST Webbook
tb	641.81	K	Joback Method
tc	809.89	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=R264641&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