2-Methylpentanal, PFBO # 1

Inchi: InChI=1S/C13H14F5NO/c1-3-4-7(2)5-19-20-6-8-9(14)11(16)13(18)12(17)10(8)15/h5,7H,
InchiKey: IOULWMZNMCBDQK-UHFFFAOYSA-N
Formula: C13H14F5NO
SMILES: CCCC(C)C=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 295.25

Physical Properties

Property code	Value	Unit	Source
hf	-1168.30	kJ/mol	Joback Method
hvap	51.37	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.321		Crippen Method
mcvol	190.670	ml/mol	McGowan Method
pc	1539.08	kPa	Joback Method
rinpol	1387.00		NIST Webbook
rinpol	1387.00		NIST Webbook
ripol	1647.00		NIST Webbook
ripol	1647.00		NIST Webbook
tb	643.43	K	Joback Method
tc	822.07	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R574775&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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