3-Methylbutanal, PFBO # 1

Inchi: InChI=1S/C12H12F5NO/c1-6(2)3-4-18-19-5-7-8(13)10(15)12(17)11(16)9(7)14/h4,6H,3,5
InchiKey: HNAOVROTLABYSA-UHFFFAOYSA-N
Formula: C12H12F5NO
SMILES: CC(C)CC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 281.22

Physical Properties

Property code	Value	Unit	Source
hf	-1147.66	kJ/mol	Joback Method
hvap	49.14	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	3.931		Crippen Method
mcvol	176.580	ml/mol	McGowan Method
pc	1661.90	kPa	Joback Method
rinpol	1321.00		NIST Webbook
rinpol	1321.00		NIST Webbook
ripol	1599.00		NIST Webbook
ripol	1599.00		NIST Webbook
tb	620.55	K	Joback Method
tc	800.34	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=R574993&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature