Propanal, 3-methylthio, PFBO # 1

Inchi: InChI=1S/C11H10F5NOS/c1-19-3-2-17-5-18-4-6-7(12)9(14)11(16)10(15)8(6)13/h5H,2-4
InchiKey: PFCXJELCINRJIV-UHFFFAOYSA-N
Formula: C11H10F5NOS
SMILES: CSCCN=COCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 299.26

Physical Properties

Property code	Value	Unit	Source
hf	-1079.87	kJ/mol	Joback Method
hvap	54.12	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.290		Crippen Method
mcvol	178.840	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	1587.00		NIST Webbook
rinpol	1587.00		NIST Webbook
ripol	2147.00		NIST Webbook
tb	666.89	K	Joback Method
tc	859.98	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=R575847&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