Hexanal, 3-methylthio, PFBO # 1

Inchi: InChI=1S/C14H16F5NOS/c1-3-4-8(22-2)5-6-20-21-7-9-10(15)12(17)14(19)13(18)11(9)16
InchiKey: VVWJYXZORWPCEK-UHFFFAOYSA-N
Formula: C14H16F5NOS
SMILES: CCCC(CC=NOCc1c(F)c(F)c(F)c(F)c1F)SC
Mol. weight [g/mol]: 341.34

Physical Properties

Property code	Value	Unit	Source
hf	-1147.07	kJ/mol	Joback Method
hvap	60.41	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	4.806		Crippen Method
mcvol	221.110	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	1779.00		NIST Webbook
rinpol	1779.00		NIST Webbook
ripol	2250.00		NIST Webbook
ripol	2250.00		NIST Webbook
tb	735.09	K	Joback Method
tc	926.83	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R575783&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