2-Butanone, 3-methylthio, PFBO # 1

Inchi: InChI=1S/C12H12F5NOS/c1-5(6(2)20-3)18-19-4-7-8(13)10(15)12(17)11(16)9(7)14/h6H,4

InchiKey: IBRSSDPLIBYCFA-UHFFFAOYSA-N

Formula: C12H12F5NOS

SMILES: CSC(C)C(C)=NOCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 313.29

Physical Properties

Property code	Value	Unit	Source
hf	-1115.58	kJ/mol	Joback Method
hvap	56.04	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.026		Crippen Method
mcvol	192.930	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
rinpol	1393.00		NIST Webbook
ripol	1894.00		NIST Webbook
tb	689.21	K	Joback Method
tc	886.19	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R574651&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

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