2-Butanone, 4-methylthio, PFBO # 1

Inchi: InChI=1S/C12H12F5NOS/c1-6(3-4-20-2)18-19-5-7-8(13)10(15)12(17)11(16)9(7)14/h3-5H
InchiKey: RZTPUHVTRNLFEF-UHFFFAOYSA-N
Formula: C12H12F5NOS
SMILES: CSCCC(C)=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 313.29

Physical Properties

Property code	Value	Unit	Source
hf	-1110.30	kJ/mol	Joback Method
hvap	56.43	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.028		Crippen Method
mcvol	192.930	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	1601.00		NIST Webbook
ripol	2085.00		NIST Webbook
ripol	2085.00		NIST Webbook
tb	689.65	K	Joback Method
tc	883.54	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=R574691&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