3-Mercapto-3-methyl-2-pentanone, PFBO # 1

Inchi: InChI=1S/C13H14F5NOS/c1-4-13(3,21)6(2)19-20-5-7-8(14)10(16)12(18)11(17)9(7)15/h2
InchiKey: NGVBKSFWBDKEDD-UHFFFAOYSA-N
Formula: C13H14F5NOS
SMILES: CCC(C)(S)C(C)=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 327.31

Physical Properties

Property code	Value	Unit	Source
hf	-1143.08	kJ/mol	Joback Method
hvap	57.28	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	4.373		Crippen Method
mcvol	207.020	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	1686.00		NIST Webbook
ripol	1995.00		NIST Webbook
ripol	1995.00		NIST Webbook
tb	703.38	K	Joback Method
tc	904.23	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R574973&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