3-Mercapto-2-pentanone, PFBO # 2

Inchi: InChI=1S/C12H12F5NOS/c1-3-7(20)5(2)18-19-4-6-8(13)10(15)12(17)11(16)9(6)14/h7,20
InchiKey: NTTWHZVTGURFAX-UHFFFAOYSA-N
Formula: C12H12F5NOS
SMILES: CCC(S)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	-1118.97	kJ/mol	Joback Method
hvap	55.96	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	3.983		Crippen Method
mcvol	192.930	ml/mol	McGowan Method
pc	1759.49	kPa	Joback Method
rinpol	1535.00		NIST Webbook
tb	683.29	K	Joback Method
tc	880.39	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R574968&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature