3-Mercapto-2-butanone, PFBO # 1

Inchi: InChI=1S/C11H10F5NOS/c1-4(5(2)19)17-18-3-6-7(12)9(14)11(16)10(15)8(6)13/h5,19H,3
InchiKey: HQSITFOAMQIFJY-UHFFFAOYSA-N
Formula: C11H10F5NOS
SMILES: CC(=NOCc1c(F)c(F)c(F)c(F)c1F)C(C)S
Mol. weight [g/mol]: 299.26

Physical Properties

Property code	Value	Unit	Source
hf	-1098.33	kJ/mol	Joback Method
hvap	53.73	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	3.593		Crippen Method
mcvol	178.840	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	1466.00		NIST Webbook
ripol	1909.00		NIST Webbook
ripol	1909.00		NIST Webbook
tb	660.41	K	Joback Method
tc	859.75	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=R574933&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