Acetone, methylthio, PFBO # 1

Inchi: InChI=1S/C10H8F5NOS/c1-4(3-18)16-17-2-5-6(11)8(13)10(15)9(14)7(5)12/h18H,2-3H2,
InchiKey: SZRMFYIXEKJNFX-UHFFFAOYSA-N
Formula: C10H8F5NOS
SMILES: CC(CS)=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 285.23

Physical Properties

Property code	Value	Unit	Source
hf	-1072.41	kJ/mol	Joback Method
hvap	51.90	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.204		Crippen Method
mcvol	164.750	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1493.00		NIST Webbook
rinpol	1493.00		NIST Webbook
tb	637.97	K	Joback Method
tc	836.25	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=R576068&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

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