Tetrahydrothiophen-3-one, 2-methyl, PFBO # 2

Inchi: InChI=1S/C12H10F5NOS/c1-5-7(2-3-20-5)18-19-4-6-8(13)10(15)12(17)11(16)9(6)14/h5H
InchiKey: UMRDBTHTODYARP-UHFFFAOYSA-N
Formula: C12H10F5NOS
SMILES: CC1SCCC1=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 311.27

Physical Properties

Property code	Value	Unit	Source
hf	-1077.83	kJ/mol	Joback Method
hvap	56.43	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	3.780		Crippen Method
mcvol	182.070	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
rinpol	1663.00		NIST Webbook
ripol	2182.00		NIST Webbook
ripol	2182.00		NIST Webbook
tb	686.58	K	Joback Method
tc	892.24	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=R575916&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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