Phosphinodithioic acid, bis(trifluoromethyl) ester

Inchi: InChI=1S/C2HF6PS2/c3-1(4,5)10-9-11-2(6,7)8/h9H
InchiKey: VLJMMPNLEDMJJL-UHFFFAOYSA-N
Formula: C2HF6PS2
SMILES: FC(F)(F)SPSC(F)(F)F
Mol. weight [g/mol]: 234.12
CAS: 18799-75-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.77		Crippen Method
logp	4.001		Crippen Method
mcvol	102.820	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	41.90	kJ/mol	280.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18799752&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hsubt: Enthalpy of sublimation at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume