

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
mcpvol	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/ci9903071>
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

Latest version available from:

<https://www.cheméo.com/cid/98-687-2/Phosphinodithioic-acid-bis-trifluoromethyl-ester.pdf>

Generated by Cheméo on 2024-04-25 20:52:17.791903615 +0000 UTC m=+16367586.712480930.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.