Phosphorus monosulfide

Inchi: InChI=1S/PS/c1-2
InchiKey: VKCLPVFDVVKEKU-UHFFFAOYSA-N
Formula: PS
SMILES: [P]=S
Mol. weight [g/mol]: 63.04
CAS: 12281-36-6

Physical Properties

Property code	Value	Unit	Source
affp	698.00	kJ/mol	NIST Webbook
basg	665.50	kJ/mol	NIST Webbook
ie	9.00	eV	NIST Webbook
log10ws	3.57		Crippen Method
logp	0.859		Crippen Method
mcvol	41.220	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C12281366&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume