Diphosphoric acid

Inchi: InChI=1S/H4O7P2/c1-8(2,3)7-9(4,5)6/h(H2,1,2,3)(H2,4,5,6)
InchiKey: XPPKVPWEQAFLFU-UHFFFAOYSA-N
Formula: H4O7P2
SMILES: O=P(O)(O)OP(=O)(O)O
Mol. weight [g/mol]: 177.97
CAS: 2466-09-3

Physical Properties

Property code	Value	Unit	Source
logp	-0.812		Crippen Method
mcvol	92.870	ml/mol	McGowan Method
tf	334.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

Latest version available from:

https://www.chemeo.com/cid/102-712-7/Diphosphoric-acid.pdf

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