

Bis(trifluoromethyl)phosphine

Other names:	Bis(trifluoromethyl)phosphine
Inchi:	InChI=1S/C2HF6P/c3-1(4,5)9-2(6,7)8/h9H
InchiKey:	CJOZYRZUMSWLHJ-UHFFFAOYSA-N
Formula:	C2HF6P
SMILES:	FC(F)(F)PC(F)(F)F
Mol. weight [g/mol]:	169.99

Physical Properties

Property code	Value	Unit	Source
ie	11.50	eV	NIST Webbook
ie	11.51	eV	NIST Webbook
logp	2.705		Crippen Method
mcvol	70.120	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C460968&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/88-167-0/Bis-trifluoromethyl-phosphine.pdf>

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