Phosphonic acid, 4-morpholinyl-, dimethyl ester

Other names: Dimethyl morpholinophosphonate
Phosphonic acid, 4-morpholinyl-, dimethyl ester
Phosphonic acid, morpholino-, dimethyl ester
HC 1717
Morpholinophosphonic acid dimethyl ester
NCI-C54740
Dimethyl 4-morpholinylphosphonate

Inchi: InChI=1S/C6H14NO4P/c1-9-12(8,10-2)7-3-5-11-6-4-7/h3-6H2,1-2H3

InchiKey: BZXUQIDKDGGYPB-UHFFFAOYSA-N

Formula: C6H14NO4P

SMILES: COP(=O)(OC)N1CCOCC1

Mol. weight [g/mol]: 195.16

Physical Properties

Property code	Value	Unit	Source
logp	0.720		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
rinpol	1296.00		NIST Webbook
rinpol	1353.60		NIST Webbook
rinpol	1296.20		NIST Webbook
rinpol	1353.60		NIST Webbook
rinpol	1296.00		NIST Webbook
ripol	2145.40		NIST Webbook
ripol	2145.40		NIST Webbook
ripol	2145.00		NIST Webbook
ripol	2145.00		NIST Webbook

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):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C597251&Units=SI

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

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices