Cycloheptyl methylphosphonofluoridoate

Other names: Methylphosphonic acid, fluoroanhydride, cycloheptyl ester
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Inchi: InChI=1S/C8H16FO2P/c1-12(9,10)11-8-6-4-2-3-5-7-8/h8H,2-7H2,1H3
InchiKey: FLEZPAFIBXHSRI-UHFFFAOYSA-N
Formula: C8H16FO2P
SMILES: CP(=O)(F)OC1CCCCCC1
Mol. weight [g/mol]: 194.19

Physical Properties

Property code	Value	Unit	Source
hvap	62.17	kJ/mol	Cheméo Relay (1.0)
ie	10.15	eV	Cheméo Relay (1.0)
logp	3.518		Crippen Method
mcvol	146.690	ml/mol	McGowan Method
rinpol	1340.00		NIST Webbook
rinpol	1340.00		NIST Webbook
tb	511.14	K	Cheméo Relay (1.0)
tf	255.67	K	Cheméo Relay (1.0)

Sources

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7284835&Units=SI

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point