

4-Ethyl-2,6,7-Trioxa-1-phosphabicyclo[2.2.2]octane

Other names:	4-Ethyl-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane 1,3-Propanediol, 2-ethyl-2-(hydroxymethyl)-, cyclic phosphite (1:1) Trimethylolpropane cyclic phosphite (1:1) 2,6,7-Trioxa-1-phosphabicyclo[2.2.2]octane, 4-ethyl- 1,1,1-Trishydroxymethylpropane bicyclic phosphite 4-Aethyl-1-phospha-2,6,7-trioxabicyclo(2.2.2)octan 4-Ethyl-1-phospha-2,6,7-trioxabicyclo(2.2.2)octane 2-(Hydroxymethyl)-2-ethyl-1,3-propanediol, cyclic phosphite (1:1) NSC 127561 4-Ethyl-2.6.7-trioxa-1-phospha-bicyclo[2.2.2]octane Ethyl bicyclic phosphite
Inchi:	InChI=1S/C6H11O3P/c1-2-6-3-7-10(8-4-6)9-5-6/h2-5H2,1H3
InchiKey:	QRUSNTDXJQBKBI-UHFFFAOYSA-N
Formula:	C6H11O3P
SMILES:	CCC12COP(OC1)OC2
Mol. weight [g/mol]:	162.13

Physical Properties

Property code	Value	Unit	Source
ie	9.76	eV	Cheméo Relay (1.0)
logp	1.687		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
rinpol	1221.00		NIST Webbook
rinpol	1221.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.00 ± 1.00	K	0.30	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C824113&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
rinpol:	Non-polar retention indices
tbrp:	Boiling point at reduced pressure

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