

Methylphosphonic acid, dipropyl ester

Other names:	Methylphosphonic acid, dipropyl ester
Inchi:	InChI=1S/C7H17O3P/c1-4-6-9-11(3,8)10-7-5-2/h4-7H2,1-3H3
InchiKey:	NRMHUSQXOMWJGD-UHFFFAOYSA-N
Formula:	C7H17O3P
SMILES:	CCCOP(C)(=O)OCCC
Mol. weight [g/mol]:	180.18

Physical Properties

Property code	Value	Unit	Source
af	0.5228		Cheméo Relay (1.0)
gf	-345.82	kJ/mol	Cheméo Relay (1.0, beta)
hf	-705.53	kJ/mol	Cheméo Relay (1.0)
hvap	62.50	kJ/mol	Cheméo Relay (1.0)
ie	9.99	eV	Cheméo Relay (1.0)
log10ws	-0.89		Cheméo Relay (1.0)
logp	2.663		Crippen Method
mcvol	147.560	ml/mol	McGowan Method
pc	2440.64	kPa	Cheméo Relay (1.0, beta)
tb	500.68	K	Cheméo Relay (1.0)
tc	624.41	K	Cheméo Relay (1.0)
tf	206.45	K	Cheméo Relay (1.0)
vc	0.572	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C6410566&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

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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