

# Isofluorophate

<b>Other names:</b>	DFP Diflupyl Difluorophate Diisopropoxyphosphoryl fluoride Diisopropyl fluorophosphate Diisopropyl fluorophosphonate Diisopropyl phosphofluoridate Diisopropyl phosphorofluoridate Diisopropylfluorfosfat Diisopropylfluorophosphoric acid ester Diisopropylfluorphosphorsaeureester Disiopropyl fluorophosphonate Dyflos EA 1152 Floropryl Fluophosphoric acid, diisopropyl ester Fluorodiisopropyl phosphate Fluorophosphoric acid, diisopropyl ester Fluoropryl Fluostigmine Fluropryl Isofluorophate Isofluorophate Isopropyl fluophosphate Isopropyl phosphorofluoridate Neoglaucit O,O'-Diisopropyl phosphoryl fluoride O,O-Diisopropyl fluorophosphate PF-3 Phosphorofluoridic acid, bis(1-methylethyl) ester Phosphorofluoridic acid, diisopropyl ester Rcra waste number P043 T-1703 TL 466
<b>Inchi:</b>	InChI=1S/C6H14FO3P/c1-5(2)9-11(7,8)10-6(3)4/h5-6H,1-4H3
<b>InchiKey:</b>	MUCZHBLJLSDCSD-UHFFFAOYSA-N
<b>Formula:</b>	C6H14FO3P
<b>SMILES:</b>	CC(C)OP(=O)(F)OC(C)C
<b>Mol. weight [g/mol]:</b>	184.15
<b>CAS:</b>	55-91-4

# Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	2.914		Crippen Method
mcpvol	135.240	ml/mol	McGowan Method
ripol	927.00		NIST Webbook
ripol	926.00		NIST Webbook
ripol	929.00		NIST Webbook
ripol	1342.00		NIST Webbook
ripol	1341.00		NIST Webbook
ripol	1342.40		NIST Webbook
ripol	1342.00		NIST Webbook

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	29.40	kJ/mol	310.50	NIST Webbook

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.26747e+01
Coeff. B	-7.70123e+03
Temperature range (K), min.	344.00
Temperature range (K), max.	443.54

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C55914&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55914&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pvap:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices

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