

Octicizer

Other names:	(2-Ethylhexyl)-difenylfosfat 1-Hexanol, 2-ethyl-, ester with diphenyl phosphate 2-Ethyl-1-hexanol ester with diphenyl phosphate 2-Ethylhexyl diphenyl ester of phosphoric acid 2-Ethylhexyl diphenyl ester phosphoric acid 2-Ethylhexyl diphenyl phosphate Diphenyl 2-ethylhexyl phosphate Disflamoll DPO Phosflex 362 Phosphoric acid diphenyl 2-ethylhexyl ester Phosphoric acid, 2-ethylhexyl diphenyl ester Sancticiser 141 Sancticizer 141 Santicizer 141
Inchi:	InChI=1S/C20H27O4P/c1-3-5-12-18(4-2)17-22-25(21,23-19-13-8-6-9-14-19)24-20-15-10
InchiKey:	CGSLYBDCEGBZCG-UHFFFAOYSA-N
Formula:	C20H27O4P
SMILES:	CCCCC(CC)COP(=O)(Oc1ccccc1)Oc1ccccc1
Mol. weight [g/mol]:	362.40
CAS:	1241-94-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.98		Crippen Method
logp	6.485		Crippen Method
mcvol	289.080	ml/mol	McGowan Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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pvap	8.90e-08	kPa	298.00	Determination of Vapor Pressures for Organophosphate Esters
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Sources

Determination of Vapor Pressures for Organophosphate Esters: McGowan Method:

<https://www.doi.org/10.1021/je401026a>

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1241947&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/36-724-8/Octicizer.pdf>

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