

Ethanol, 2-butoxy-, phosphate (3:1)

Other names:

19040-50-7
2-Butoxy-ethanol phosphate (3:1)
2-Butoxyethanol phosphate
31227-66-4
Amgard TBEP
Ethanol, 2-butoxy-, 1,1',1''-phosphate
KP 140
Kronitex KP-140
NSC 4839
Phosflex T-bep
Phosphoric acid, tri-(2-butoxyethyl) ester
Phosphoric acid, tributoxyethyl ester
Phosphoric acid, tris(2-butoxyethyl) ester
TBEP
Tri(2-butoxyethanol)phosphate
Tri(2-butoxyethyl) phosphate
Tri(butoxyethyl) phosphate
Tributyl cellosolve phosphate
Tris(2-butoxyethyl) phosphate
Tris(2-butoxyethyl)ester phosphoric acid
Tris(butoxyethyl) phosphate
Tris-(2-butoxyethyl)fosfat

Inchi:

InChI=1S/C18H39O7P/c1-4-7-10-20-13-16-23-26(19,24-17-14-21-11-8-5-2)25-18-15-22-

InchiKey:

WTLBZVNBAKMVDP-UHFFFAOYSA-N

Formula:

C18H39O7P

SMILES:

CCCCOCCOP(=O)(OCCOCCCC)OCCOCCCC

Mol. weight [g/mol]:

398.47

CAS:

78-51-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Crippen Method
logp	4.594		Crippen Method
mcvol	326.030	ml/mol	McGowan Method
rinpol	2363.00		NIST Webbook
rinpol	2421.00		NIST Webbook

rropol	2360.00	NIST Webbook
rropol	2364.00	NIST Webbook
rropol	2363.00	NIST Webbook
rropol	2363.00	NIST Webbook
rropol	2363.00	NIST Webbook
rropol	397.30	NIST Webbook
rropol	2364.00	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	4.90e-08	kPa	298.00	Determination of Vapor Pressures for Organophosphate Esters

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination of Vapor Pressures for Organophosphate Esters:	https://www.doi.org/10.1021/je401026a
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78513&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

Legend

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

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