

Phosphoric acid, tris(2-ethylhexyl) ester

Other names:

1-Hexanol, 2-ethyl-, phosphate
2-Ethyl-1-hexanol phosphate
2-Ethylhexanol phosphate (3:1)
2-Ethylhexanol, phosphate triester
Amgard TOF
Disflamoll TOF
Flexol TOF
Flexol plasticizer TOF
Kronitex TOF
NCI-C54751
NSC 407921
Phosphoric acid, tris(ethylhexyl) ester
TOF
Tri(ethylhexyl) phosphate
Trioctyl phosphate
Tris(ethylhexyl) phosphate
Tris-(2-ethylhexyl)fosfat
tri(2-ethylhexyl) phosphate
tris(2-ethylhexyl) phosphate

Inchi:

InChI=1S/C24H51O4P/c1-7-13-16-22(10-4)19-26-29(25,27-20-23(11-5)17-14-8-2)28-21-

InchiKey:

GTVWRXDRKAHEAD-UHFFFAOYSA-N

Formula:

C24H51O4P

SMILES:

CCCCC(CC)COP(=O)(OCC(CC)CCCC)OCC(CC)CCCC

Mol. weight [g/mol]:

434.63

CAS:

78-42-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.67		Crippen Method
logp	8.793		Crippen Method
mcvol	392.960	ml/mol	McGowan Method
rinpol	2463.00		NIST Webbook
rinpol	2463.00		NIST Webbook
rinpol	2448.00		NIST Webbook
rinpol	2448.00		NIST Webbook
rinpol	2463.00		NIST Webbook
rinpol	2463.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
dvisc	0.0140870	Paxs	293.15	Densities and Viscosities of Binary Mixtures of Tris(2-ethylhexyl) Phosphate + Cyclohexane or n-Hexane at T) (293.15, 298.15, and 303.15) K and p) 0.1 MPa
dvisc	0.0116150	Paxs	298.15	Densities and Viscosities of Binary Mixtures of Tris(2-ethylhexyl) Phosphate + Cyclohexane or n-Hexane at T) (293.15, 298.15, and 303.15) K and p) 0.1 MPa
dvisc	0.0097080	Paxs	303.15	Densities and Viscosities of Binary Mixtures of Tris(2-ethylhexyl) Phosphate + Cyclohexane or n-Hexane at T) (293.15, 298.15, and 303.15) K and p) 0.1 MPa
pvap	2.10e-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: Densities and Viscosities of Binary Mixtures of Tris(2-ethylhexyl) Phosphate + Cyclohexane or n-Hexane at T) (293.15, 298.15, and 303.15) K and p) 0.1 MPa:

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

<https://www.doi.org/10.1021/je8006138>

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C78422&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

dvisc:	Dynamic viscosity
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
tf:	Normal melting (fusion) point

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