

tri-n-Hexylphosphate

Other names:	tri-n-hexyl phosphate trihexyl phosphate
Inchi:	InChI=1S/C18H39O4P/c1-4-7-10-13-16-20-23(19,21-17-14-11-8-5-2)22-18-15-12-9-6-3/h
InchiKey:	SFENPMLASUEABX-UHFFFAOYSA-N
Formula:	C18H39O4P
SMILES:	CCCCCOP(=O)(OCCCCC)OCCCCC
Mol. weight [g/mol]:	350.47
CAS:	2528-39-4

Physical Properties

Property code	Value	Unit	Source
hvap	104.80	kJ/mol	NIST Webbook
hvap	104.90	kJ/mol	NIST Webbook
log10ws	-7.88		Crippen Method
logp	6.885		Crippen Method
mcvol	308.420	ml/mol	McGowan Method
rinpol	2174.00		NIST Webbook
rinpol	2228.00		NIST Webbook
rinpol	2174.00		NIST Webbook
tb	639.27	K	Estimation of Normal Boiling points of Trialkyl Phosphates using Retention indices by Gas Chromatography

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	104.91	kJ/mol	298.15	Measurement of enthalpies of vaporization of trialkyl phosphates using correlation gas chromatography

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement of enthalpies of vaporization of trialkyl phosphates	https://www.doi.org/10.1016/j.tca.2007.10.007
Estimation of Normal Boiling Points of Trialkyl Phosphates using Retention Indices by Gas Chromatography:	https://www.doi.org/10.1016/j.tca.2010.07.032
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2528394&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

h_{vap}:	Enthalpy of vaporization at standard conditions
h_{vapt}:	Enthalpy of vaporization at a given temperature
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

Latest version available from:

<https://www.chemeo.com/cid/99-278-5/tri-n-Hexylphosphate.pdf>

Generated by Cheméo on 2024-04-26 17:15:55.160024618 +0000 UTC m=+16441004.080601929.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.