

Trihexyl phosphate

Other names:	tri-n-hexyl 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]:	350.48

Physical Properties

Property code	Value	Unit	Source
af	0.9456		Cheméo Relay (1.0)
gf	-351.74	kJ/mol	Cheméo Relay (1.0, beta)
hf	-1084.99	kJ/mol	Cheméo Relay (1.0)
hvap	104.80	kJ/mol	NIST Webbook
hvap	104.90	kJ/mol	NIST Webbook
ie	10.07	eV	Cheméo Relay (1.0)
log10ws	-5.26		Cheméo Relay (1.0)
logp	6.885		Crippen Method
mcvol	308.420	ml/mol	McGowan Method
pc	1257.53	kPa	Cheméo Relay (1.0, beta)
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
tc	764.54	K	Cheméo Relay (1.0)
tf	230.56	K	Cheméo Relay (1.0)
vc	1.206	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Measurement of enthalpies of vaporization of trialkyl phosphates	https://www.doi.org/10.1016/j.tca.2007.10.007
Estimation of Normal Boiling Point of Trialkyl Phosphates using Retention Indices by Gas Chromatography	https://www.doi.org/10.1016/j.tca.2010.07.032
NIST Webbook	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2528394&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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