Tri-n-octyl phosphate

Other names: Trioctyl phosphate
tri-n-Octylphosphate
Tris(n-octyl) phosphate
Inchi: InChI=1S/C24H51O4P/c1-4-7-10-13-16-19-22-26-29(25,27-23-20-17-14-11-8-5-2)28-24-
InchiKey: WVPGXJOLGGFBCR-UHFFFAOYSA-N
Formula: C24H51O4P
SMILES: CCCCCCCCOP(=O)(OCCCCCCCC)OCCCCCCCC
Mol. weight [g/mol]: 434.64

Physical Properties

Property code	Value	Unit	Source
af	1.1558		Cheméo Relay (1.0)
gf	-299.68	kJ/mol	Cheméo Relay (1.0, beta)
hf	-1200.85	kJ/mol	Cheméo Relay (1.0)
hvap	124.46	kJ/mol	Cheméo Relay (1.0)
ie	10.11	eV	Cheméo Relay (1.0)
log10ws	-7.41		Cheméo Relay (1.0)
logp	9.226		Crippen Method
mcvol	392.960	ml/mol	McGowan Method
pc	777.52	kPa	Cheméo Relay (1.0, beta)
rinpol	2476.00		NIST Webbook
rinpol	2445.00		NIST Webbook
rinpol	2445.00		NIST Webbook
rinpol	2445.00		NIST Webbook
tb	668.12	K	Cheméo Relay (1.0)
tc	814.52	K	Cheméo Relay (1.0)
tf	263.14	K	Cheméo Relay (1.0)
vc	1.541	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1806548&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

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
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