DIOCTYL PHENYLPHOSPHONATE

Other names:	di-n-Octyl phenylphosphonate
	Phosphonic acid, phenyl-, dioctyl ester
	Benzenephosphonic acid, dioctyl ester
	Phenylphosphonic acid dioctyl ester
Inchi:	InChI=1S/C22H39O3P/c1-3-5-7-9-11-16-20-24-26(23,22-18-14-13-15-19-22)25-21-17-12
InchiKey:	HAKMAMKAFTZXOZ-UHFFFAOYSA-N
Formula:	C22H39O3P
SMILES:	CCCCCCCCOP(=O)(OCCCCCCCC)c1ccccc1
Mol. weight [g/mol]:	382.52

Physical Properties

Property code	Value	Unit	Source
af	0.9984		Cheméo Relay (1.0)
hvap	115.32	kJ/mol	Cheméo Relay (1.0)
ie	9.31	eV	Cheméo Relay (1.0)
log10ws	-6.30		Cheméo Relay (1.0)
logp	7.259		Crippen Method
mcvol	335.150	ml/mol	McGowan Method
pc	1097.72	kPa	Cheméo Relay (1.0, beta)
tb	664.17	K	Cheméo Relay (1.0)
tc	850.60	K	Cheméo Relay (1.0)
tf	275.99	K	Cheméo Relay (1.0)
vc	1.265	m3/kmol	Cheméo Relay (1.0)

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1754478&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume