

diphenyl hydrogen phosphate

Inchi:	InChI=1S/C12H11O4P/c13-17(14,15-11-7-3-1-4-8-11)16-12-9-5-2-6-10-12/h1-10H,(H,13
InchiKey:	ASMQGLCHMVWBQR-UHFFFAOYSA-N
Formula:	C12H11O4P
SMILES:	O=P(O)(Oc1ccccc1)Oc1ccccc1
Mol. weight [g/mol]:	250.19
CAS:	838-85-7

Physical Properties

Property code	Value	Unit	Source
af	0.8290		Cheméo Relay (1.0)
hf	-496.59	kJ/mol	Cheméo Relay (1.0)
hvap	102.68	kJ/mol	Cheméo Relay (1.0)
ie	9.05	eV	Cheméo Relay (1.0)
log10ws	-2.61		Cheméo Relay (1.0)
logp	3.245		Crippen Method
mcvol	176.360	ml/mol	McGowan Method
pc	2701.64	kPa	Cheméo Relay (1.0, beta)
tb	595.32	K	Cheméo Relay (1.0)
tc	894.67	K	Cheméo Relay (1.0)
tf	339.90	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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