

1,3 Diphenylisobenzofuran

Other names:	Diphenylisobenzofuran 1,4-Diphenyl-2,3-benzofuran Isobenzofuran, 1,3-diphenyl- 1,3-Diphenylbenzo[c]furan
Inchi:	InChI=1S/C20H14O/c1-3-9-15(10-4-1)19-17-13-7-8-14-18(17)20(21-19)16-11-5-2-6-12-1
InchiKey:	ZKSVYBRJSMBDMV-UHFFFAOYSA-N
Formula:	C20H14O
SMILES:	<chem>c1ccc(-c2oc(-c3ccccc3)c3ccccc23)cc1</chem>
Mol. weight [g/mol]:	270.32
CAS:	5471-63-6

Physical Properties

Property code	Value	Unit	Source
chs	-9952.00 ± 9.10	kJ/mol	NIST Webbook
hf	203.00 ± 10.00	kJ/mol	NIST Webbook
hfs	81.00 ± 9.20	kJ/mol	NIST Webbook
hsub	121.50 ± 0.90	kJ/mol	NIST Webbook
hsub	122.00	kJ/mol	NIST Webbook
log10ws	-12.22		Crippen Method
logp	5.767		Crippen Method
mvol	212.090	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5471636&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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