5H-Dibenzo[a,d]cyclohepten-5-one

Other names:	2,3:6,7-Dibenzosuberen-4-on-1
	2,3:6,7-Dibenzotropone
	5H-Dibenzo[a,d]cycloheptenone
	Dibenzosuberenone
	Dibenzosuberenone-5
	5-Dibenzosuberenone
	Dibenzo(a,d)cyclohepten-5-one
	NSC 86151
	dibenzo[b,f]cyclohepten-1-one
Inchi:	InChI=1S/C15H10O/c16-15-13-7-3-1-5-11(13)9-10-12-6-2-4-8-14(12)15/h1-10H
InchiKey:	SNVTZAIYUGUKNI-UHFFFAOYSA-N
Formula:	C15H10O
SMILES:	O=c1c2ccccc2ccc2ccccc12
Mol. weight [g/mol]:	206.24
CAS:	2222-33-5

Physical Properties

Property code	Value	Unit	Source
chs	-7326.00 ± 27.00	kJ/mol	NIST Webbook
hfs	-7.00 ± 27.00	kJ/mol	NIST Webbook
ie	8.06 ± 0.03	eV	NIST Webbook
log10ws	-4.50		Crippen Method
logp	3.353		Crippen Method
mcvol	161.100	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C2222335&Units=SI

Legend

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