6,19-Methanobenzocyclooctadecen-21-one

Inchi: InChI=1S/C23H30O/c24-23-21-15-9-7-5-3-1-2-4-6-8-10-16-22(23)18-20-14-12-11-13-19(
InchiKey: LRURKHXGUOCKOP-UHFFFAOYSA-N
Formula: C23H30O
SMILES: O=c1c2cc3ccccc3cc1CCCCCCCCCCCC2
Mol. weight [g/mol]: 322.48
CAS: 25401-43-8

Physical Properties

Property code	Value	Unit	Source
chs	-13075.00 ± 11.00	kJ/mol	NIST Webbook
hf	-160.00 ± 15.00	kJ/mol	NIST Webbook
hfs	-263.00 ± 11.00	kJ/mol	NIST Webbook
ie	8.15 ± 0.03	eV	NIST Webbook
log10ws	-7.55		Crippen Method
logp	6.200		Crippen Method
mcvol	282.420	ml/mol	McGowan Method

Sources

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=C25401438&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
hf: Enthalpy of formation at standard conditions
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