9,10-Dehydrophenanthrene

Inchi: InChI=1S/C14H8/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h1-8H
InchiKey: GGLLFYKEZTUKRK-UHFFFAOYSA-N
Formula: C14H8
SMILES: c1c2ccccc2c2ccccc2c#1
Mol. weight [g/mol]: 176.21
CAS: 7048-96-6

Physical Properties

Property code	Value	Unit	Source
hf	600.00 ± 40.00	kJ/mol	NIST Webbook
log10ws	-4.45		Crippen Method
logp	3.593		Crippen Method
mcvol	141.140	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7048966&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.