[2,3-d]-Furocycloheptatrienone

Inchi: InChI=1S/C9H6O2/c10-9-3-1-7-5-11-6-8(7)2-4-9/h1-6H
InchiKey: UDTGOPLYKGNTOA-UHFFFAOYSA-N
Formula: C9H6O2
SMILES: O=c1ccc2cocc2cc1
Mol. weight [g/mol]: 146.14
CAS: 18895-06-2

Physical Properties

Property code	Value	Unit	Source
ie	8.65	eV	NIST Webbook
log10ws	-6.43		Crippen Method
logp	1.793		Crippen Method
mcvol	106.190	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18895062&Units=SI
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

Legend

ie: Ionization energy
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.