

Indeno[2,1-b]oxine, 2-phenyl-

Other names:	2-Phenylindeno[2,1-b]pyran
Inchi:	InChI=1S/C18H12O/c1-2-6-13(7-3-1)17-11-10-16-15-9-5-4-8-14(15)12-18(16)19-17/h1-1
InchiKey:	UTGHTKDYFKLHGL-UHFFFAOYSA-N
Formula:	C18H12O
SMILES:	<chem>c1ccc(-c2ccc3c4ccccc4cc-3o2)cc1</chem>
Mol. weight [g/mol]:	244.29
CAS:	10435-67-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.63		Crippen Method
logp	5.205		Crippen Method
mcpvol	188.210	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	132.80	kJ/mol	409.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10435673&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hsubt: Enthalpy of sublimation at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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