3-BENZOYLINDOLE

Other names:	3-Benzoylindole
	Ketone, indol-3-yl phenyl
	Methanone, 1H-indol-3-ylphenyl-
Inchi:	InChI=1S/C15H11NO/c17-15(11-6-2-1-3-7-11)13-10-16-14-9-5-4-8-12(13)14/h1-10,16H
InchiKey:	ADHQLIGSIQGNBW-UHFFFAOYSA-N
Formula:	C15H11NO
SMILES:	O=C(c1ccccc1)c1c[nH]c2ccccc12
Mol. weight [g/mol]:	221.26

Physical Properties

Property code	Value	Unit	Source
hf	106.80	kJ/mol	Cheméo Relay (1.0)
hvap	107.35	kJ/mol	Cheméo Relay (1.0)
ie	8.03	eV	Cheméo Relay (1.0)
log10ws	-4.27		Cheméo Relay (1.0)
logp	2.917		Crippen Method
mcvol	171.080	ml/mol	McGowan Method
pc	3320.69	kPa	Cheméo Relay (1.0, beta)
tb	653.19	K	Cheméo Relay (1.0)
tc	985.46	K	Cheméo Relay (1.0)
tf	433.76	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15224256&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point