Ketone, phenyl pyrrol-2-yl

Inchi: InChI=1S/C11H9NO/c13-11(10-7-4-8-12-10)9-5-2-1-3-6-9/h1-8,12H
InchiKey: NFGGQMYSOLVBLF-UHFFFAOYSA-N
Formula: C11H9NO
SMILES: O=C(c1ccccc1)c1ccc[nH]1
Mol. weight [g/mol]: 171.20
CAS: 7697-46-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	1.764		Crippen Method
mcvol	134.180	ml/mol	McGowan Method
tb	578.00	K	NIST Webbook
tf	352.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	403.00	K	0.01	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7697463&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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point