Quinoline, 2-phenyl-

Other names:	«alpha»-Phenylquinoline
	2-Phenylquinoline
Inchi:	InChI=1S/C15H11N/c1-2-6-12(7-3-1)15-11-10-13-8-4-5-9-14(13)16-15/h1-11H
InchiKey:	FSEXLNMNADBYJU-UHFFFAOYSA-N
Formula:	C15H11N
SMILES:	c1ccc(-c2ccc3ccccc3n2)cc1
Mol. weight [g/mol]:	205.25
CAS:	612-96-4

Physical Properties

Property code	Value	Unit	Source
hsub	105.40 ± 0.90	kJ/mol	NIST Webbook
ie	8.10	eV	NIST Webbook
log10ws	-5.64		Crippen Method
logp	3.902		Crippen Method
mcvol	165.210	ml/mol	McGowan Method
rinpol	339.21		NIST Webbook
rinpol	335.06		NIST Webbook
rinpol	339.64		NIST Webbook
tf	355.90 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	103.10 ± 0.80	kJ/mol	344.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C612964&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point