1H-Indole, 2-phenyl-

Other names:	2-phenyl-1H-indole
	2-phenylindole
	Stabilizer I
	indole, 2-phenyl-
	«alpha»-Phenylindole
Inchi:	InChI=1S/C14H11N/c1-2-6-11(7-3-1)14-10-12-8-4-5-9-13(12)15-14/h1-10,15H
InchiKey:	KLLLJCACIRKBDT-UHFFFAOYSA-N
Formula:	C14H11N
SMILES:	c1ccc(-c2cc3ccccc3[nH]2)cc1
Mol. weight [g/mol]:	193.24
CAS:	948-65-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.10		Crippen Method
logp	3.353		Crippen Method
mcvol	155.420	ml/mol	McGowan Method
rinpol	347.47		NIST Webbook
rinpol	343.02		NIST Webbook
rinpol	346.18		NIST Webbook
rinpol	347.47		NIST Webbook
rinpol	347.47		NIST Webbook
tf	462.00 ± 3.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
psub	1.02e-03	kPa	382.10	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)

psub	8.85e-04	kPa	380.12	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	7.35e-04	kPa	378.15	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	5.92e-04	kPa	376.10	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	5.00e-04	kPa	374.12	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	4.12e-04	kPa	372.16	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	3.24e-04	kPa	370.10	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	2.78e-04	kPa	368.13	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	2.27e-04	kPa	366.16	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	1.76e-04	kPa	364.08	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)

psub	1.57e-04	kPa	362.11	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)	
psub	1.22e-04	kPa	360.16	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)	
psub	1.05e-03	kPa	382.10	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)	
psub	8.68e-04	kPa	380.12	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)	
psub	7.01e-04	kPa	378.15	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)	
psub	5.90e-04	kPa	376.10	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)	
psub	4.91e-04	kPa	374.12	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)	
psub	3.92e-04	kPa	372.16	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)	

psub	3.31e-04	kPa	370.10	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	2.70e-04	kPa	368.13	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	2.17e-04	kPa	366.16	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	1.84e-04	kPa	364.08	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	1.49e-04	kPa	362.11	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	1.19e-04	kPa	360.16	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	1.05e-03	kPa	382.10	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	8.32e-04	kPa	380.12	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	6.93e-04	kPa	378.15	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)

psub	5.74e-04	kPa	376.10	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	4.56e-04	kPa	374.12	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	3.93e-04	kPa	372.16	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	3.25e-04	kPa	370.10	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	2.62e-04	kPa	368.13	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	2.14e-04	kPa	366.16	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	1.82e-04	kPa	364.08	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)
psub	1.55e-04	kPa	362.11	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)

psub	1.16e-04	kPa	360.16	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	523.20	K	1.30	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5):	https://www.doi.org/10.1016/j.jct.2015.01.012
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C948652&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point