1H-Indole, 2-phenyl-

Other names: 2-phenyl-1H-indole

2-phenylindole

Stabilizer I

indole, 2-phenyl-

«alpha»-Phenylindole

InChl=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	ce
psub 1.02e-03 kPa 382.10 Experiment computate energetic of 1-R-2-pheny (R = H, C C2H5	tional study ylindole CH3,

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)	

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

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

kPa 360.16 1.16e-04 psub 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

https://www.doi.org/10.1016/j.jct.2015.01.012

energetic study of 1-R-2-phenylindole (୧୯-୨୭୬୯୧୩) ମଧ୍ୟ ଅଧିକ୍ଷୟ :

http://link.springer.com/article/10.1007/BF02311772

http://webbook.nist.gov/cgi/cbook.cgi?ID=C948652&Units=SI

NIST Webbook: 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

McGowan's characteristic volume mcvol: psub: Sublimation pressure

rinpol: Non-polar retention indices

tbrp: Boiling point at reduced pressure tf: Normal melting (fusion) point

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