1H-Indole, 2,3-dimethyl-

Other names: 2,3-Dimethylindole
2,3-dimethyl-1H-indole
Indole, 2,3-dimethyl-
Inchi: InChI=1S/C10H11N/c1-7-8(2)11-10-6-4-3-5-9(7)10/h3-6,11H,1-2H3
InchiKey: PYFVEIDRTLBMHG-UHFFFAOYSA-N
Formula: C10H11N
SMILES: Cc1[nH]c2ccccc2c1C
Mol. weight [g/mol]: 145.20
CAS: 91-55-4

Physical Properties

Property code	Value	Unit	Source
chs	-5511.37 ± 0.79	kJ/mol	NIST Webbook
hfs	4.23 ± 0.96	kJ/mol	NIST Webbook
log10ws	-3.45		Crippen Method
logp	2.303		Crippen Method
mcvol	122.820	ml/mol	McGowan Method
rinpol	1490.30		NIST Webbook
rinpol	257.32		NIST Webbook
rinpol	255.48		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1490.30		NIST Webbook
ripol	2539.00		NIST Webbook
ripol	2502.00		NIST Webbook
tb	558.20	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47323e+01

Coeff. B	-4.67147e+03
Coeff. C	-9.63160e+01
Temperature range (K), min.	378.65
Temperature range (K), max.	592.18

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91554&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature