

Indoleacetic acid

Other names:	(1H-Indol-3-yl)-acetic acid 1H-Indole-3-acetic acid 2-(1H-indol-3-yl)acetic acid 2-(1H-indol-3-yl)ethanoic acid 2-(3-Indolyl)acetic acid 3-(Carboxymethyl)Indole 3-IAA 3-Indoleacetic acid 3-Indolylacetic acid Acetic acid, indolyl- GAP Heteroauxin Heteroauxine Heteroauxinhexterauxinia Hexteroauxin IAA Indol-3-ylacetic acid Indole-3-acetic acid Indolyl-3-acetic acid Indolylacetic acid Kyselina 3-indolyloctova NSC 3787 Rhizopin Rhizopon A «alpha»-IAA «alpha»-Indol-3-yl-acetic acid «beta»-IAA «beta»-Indole-3-acetic acid «beta»-Indoleacetic acid «beta»-Indolylacetic acid «omega»-Skatole carboxylic acid Â«alphaÂ»-IAA Â«alphaÂ»-Indol-3-yl-acetic acid Â«betaÂ»-IAA Â«betaÂ»-Indole-3-acetic acid Â«betaÂ»-Indoleacetic acid Â«betaÂ»-Indolylacetic acid Â«omegaÂ»-Skatole carboxylic acid
Inchi:	InChI=1S/C10H9NO2/c12-10(13)5-7-6-11-9-4-2-1-3-8(7)9/h1-4,6,11H,5H2,(H,12,13)
InchiKey:	SEOVTRFCIGRIMH-UHFFFAOYSA-N

Formula: C₁₀H₈NO₂
SMILES: O=C(O)Cc1c[nH]c2ccccc12
Mol. weight [g/mol]: 174.18
CAS: 87-51-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.05		Aqueous Solubility Prediction Method
logp	1.313		Crippen Method
mcvol	130.260	ml/mol	McGowan Method
tf	441.65	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	64.00 ± 1.50	kJ/mol	368.00	NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C87514&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Equilibrium Solubility, Model Correlation, and Solvent Effect of Aqueous Solubility Prediction Method: <https://www.doi.org/10.1021/acs.jced.8b01265>
More Sources and Reference Pure Solvents: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

Legend

hsubt: Enthalpy of sublimation at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

Latest version available from:

<https://www.cheméo.com/cid/40-884-6/Indoleacetic-acid.pdf>

Generated by Cheméo on 2025-12-05 16:36:25.216490813 +0000 UTC m=+4700782.746531477.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.