

7-ethylindole

Inchi:	InChI=1S/C10H11N/c1-2-8-4-3-5-9-6-7-11-10(8)9/h3-7,11H,2H2,1H3
InchiKey:	PIIZLMYXLYGWTN-UHFFFAOYSA-N
Formula:	C10H11N
SMILES:	CCc1cccc2cc[nH]c12
Mol. weight [g/mol]:	145.20
CAS:	22867-74-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.30		Crippen Method
logp	2.248		Crippen Method
mcvol	122.820	ml/mol	McGowan Method
rinpola	1344.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.16399e+01
Coeff. B	-3.34544e+03
Coeff. C	-8.10260e+01
Temperature range (K), min.	355.65
Temperature range (K), max.	609.67

Sources

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=R408534&Units=SI

Legend

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

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