

Indeno(1,2,3-de)isoquinoline

Inchi: InChI=1S/C15H9N/c1-2-6-12-11(5-1)13-7-3-4-10-8-16-9-14(12)15(10)13/h1-9H
InchiKey: AZEXTOPKZARAGZ-UHFFFAOYSA-N
Formula: C15H9N
SMILES: c1ccc2c(c1)-c1cccc3cncc-2c13
Mol. weight [g/mol]: 203.24
CAS: 7148-92-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.49		Crippen Method
logp	3.882		Crippen Method
mcvol	154.350	ml/mol	McGowan Method
tf	335.50 ± 0.50	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	425.50 ± 2.50	K	0.10	NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C7148927&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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