5,6,7,8-tetrahydroisoquinoline

Inchi: InChI=1S/C9H11N/c1-2-4-9-7-10-6-5-8(9)3-1/h5-7H,1-4H2
InchiKey: HTMGQIXFZMZZKD-UHFFFAOYSA-N
Formula: C9H11N
SMILES: c1cc2c(cn1)CCCC2
Mol. weight [g/mol]: 133.19
CAS: 36556-06-6

Physical Properties

Property code	Value	Unit	Source
affp	966.60	kJ/mol	NIST Webbook
basg	934.70	kJ/mol	NIST Webbook
ie	9.20	eV	NIST Webbook
log10ws	-2.74		Crippen Method
logp	1.960		Crippen Method
mcvol	113.030	ml/mol	McGowan Method
tb	491.20	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.20	K	1.70	NIST Webbook
tbrp	420.70	K	2.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36556066&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure