cis-3,7a-H-cis-5,8-H-3,5-Dimethylpyrrolizidine

Inchi: InChI=1S/C9H17N/c1-7-3-5-9-6-4-8(2)10(7)9/h7-9H,3-6H2,1-2H3
InchiKey: KNLORGMOTMPXIN-UHFFFAOYSA-N
Formula: C9H17N
SMILES: CC1CCC2CCC(C)N12
Mol. weight [g/mol]: 139.24
CAS: 56160-71-5

Physical Properties

Property code	Value	Unit	Source
chl	-5856.80 ± 2.00	kJ/mol	NIST Webbook
hf	-66.70 ± 2.60	kJ/mol	NIST Webbook
hfl	-114.40 ± 2.10	kJ/mol	NIST Webbook
hvap	47.70	kJ/mol	NIST Webbook
hvap	47.70	kJ/mol	NIST Webbook
log10ws	-2.28		Crippen Method
logp	2.022		Crippen Method
mcvol	125.930	ml/mol	McGowan Method

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=C56160715&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume