3-methyl-dihydroindole

Inchi: InChI=1S/C9H11N/c1-7-6-10-9-5-3-2-4-8(7)9/h2-5,7,10H,6H2,1H3
InchiKey: BFQARNDIMKOOQQ-UHFFFAOYSA-N
Formula: C9H11N
SMILES: CC1CNc2ccccc21
Mol. weight [g/mol]: 133.19

Physical Properties

Property code	Value	Unit	Source
gf	276.14	kJ/mol	Joback Method
hf	106.58	kJ/mol	Joback Method
hfus	20.44	kJ/mol	Joback Method
hvap	45.24	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.216		Crippen Method
mcvol	113.030	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
rinpol	1330.00		NIST Webbook
rinpol	1344.00		NIST Webbook
ripol	2060.00		NIST Webbook
ripol	2037.00		NIST Webbook
tb	492.27	K	Joback Method
tc	725.45	K	Joback Method
tf	353.10	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.67	J/mol×K	492.27	Joback Method
cpg	255.54	J/mol×K	531.13	Joback Method
cpg	269.41	J/mol×K	570.00	Joback Method
cpg	282.35	J/mol×K	608.86	Joback Method
cpg	294.40	J/mol×K	647.72	Joback Method
cpg	305.62	J/mol×K	686.59	Joback Method

cpg	316.08	J/mol×K	725.45	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R135172&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume