3-ethyl-dihydroindole

Inchi: InChI=1S/C10H13N/c1-2-8-7-11-10-6-4-3-5-9(8)10/h3-6,8,11H,2,7H2,1H3
InchiKey: AYIYBBZENMJOER-UHFFFAOYSA-N
Formula: C10H13N
SMILES: CCC1CNc2ccccc21
Mol. weight [g/mol]: 147.22

Physical Properties

Property code	Value	Unit	Source
gf	284.56	kJ/mol	Joback Method
hf	85.94	kJ/mol	Joback Method
hfus	23.03	kJ/mol	Joback Method
hvap	47.46	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.606		Crippen Method
mcvol	127.120	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	1427.00		NIST Webbook
rinpol	1437.00		NIST Webbook
ripol	2136.00		NIST Webbook
ripol	2158.00		NIST Webbook
tb	515.15	K	Joback Method
tc	744.15	K	Joback Method
tf	364.37	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.77	J/mol×K	515.15	Joback Method
cpg	300.59	J/mol×K	553.32	Joback Method
cpg	315.39	J/mol×K	591.48	Joback Method
cpg	329.21	J/mol×K	629.65	Joback Method
cpg	342.11	J/mol×K	667.82	Joback Method
cpg	354.17	J/mol×K	705.98	Joback Method

cpg	365.42	J/mol×K	744.15	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R135147&Units=SI

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