6-Hydroxy-dihydroindole

Inchi: InChI=1S/C8H9NO/c10-7-2-1-6-3-4-9-8(6)5-7/h1-2,5,9-10H,3-4H2
InchiKey: JWLQULBRUJIEHY-UHFFFAOYSA-N
Formula: C8H9NO
SMILES: Oc1ccc2c(c1)NCC2
Mol. weight [g/mol]: 135.16

Physical Properties

Property code	Value	Unit	Source
gf	120.81	kJ/mol	Joback Method
hf	-29.75	kJ/mol	Joback Method
hfus	22.57	kJ/mol	Joback Method
hvap	56.33	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.360		Crippen Method
mcvol	104.810	ml/mol	McGowan Method
pc	5627.81	kPa	Joback Method
rinpol	1544.00		NIST Webbook
tb	554.68	K	Joback Method
tc	805.47	K	Joback Method
tf	457.79	K	Joback Method
vc	0.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.17	J/mol×K	554.68	Joback Method
cpg	255.86	J/mol×K	596.48	Joback Method
cpg	266.54	J/mol×K	638.28	Joback Method
cpg	276.35	J/mol×K	680.07	Joback Method
cpg	285.42	J/mol×K	721.87	Joback Method
cpg	293.91	J/mol×K	763.67	Joback Method
cpg	301.93	J/mol×K	805.47	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=R135201&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume