1H-Isoindole, 2,3-dihydro-

Other names:	Isoindoline
	2-Azaindan
	2,3-dihydro-1H-isoindole
Inchi:	InChI=1S/C8H9N/c1-2-4-8-6-9-5-7(8)3-1/h1-4,9H,5-6H2
InchiKey:	GWVMLCQWXVFZCN-UHFFFAOYSA-N
Formula:	C8H9N
SMILES:	c1ccc2c(c1)CNC2
Mol. weight [g/mol]:	119.16
CAS:	496-12-8

Physical Properties

Property code	Value	Unit	Source
gf	275.43	kJ/mol	Joback Method
hf	147.56	kJ/mol	Joback Method
hfus	16.78	kJ/mol	Joback Method
hvap	43.32	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	1.290		Crippen Method
mcvol	98.940	ml/mol	McGowan Method
pc	4553.06	kPa	Joback Method
tb	474.06	K	Joback Method
tc	711.60	K	Joback Method
tf	346.07	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.35	J/mol×K	474.06	Joback Method
cpg	210.70	J/mol×K	513.65	Joback Method
cpg	223.07	J/mol×K	553.24	Joback Method
cpg	234.52	J/mol×K	592.83	Joback Method
cpg	245.11	J/mol×K	632.42	Joback Method
cpg	254.92	J/mol×K	672.01	Joback Method

cpg	264.02	J/mol×K	711.60	Joback Method

Sources

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=C496128&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume