

1H-Indole, octahydro-

Other names:	7-Azabicyclo[4.3.0]nonane Indoline, hexahydro- Octahydroindole Perhydroindole Perhydroindole,c&t octahydro-1H-indole
Inchi:	InChI=1S/C8H15N/c1-2-4-8-7(3-1)5-6-9-8/h7-9H,1-6H2
InchiKey:	PDELQDSYLBPLPQO-UHFFFAOYSA-N
Formula:	C8H15N
SMILES:	C1CCC2NCCC2C1
Mol. weight [g/mol]:	125.21
CAS:	4375-14-8

Physical Properties

Property code	Value	Unit	Source
gf	189.39	kJ/mol	Joback Method
hf	-43.52	kJ/mol	Joback Method
hfus	16.04	kJ/mol	Joback Method
hvap	40.50	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.538		Crippen Method
mcvol	111.840	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
rinpol	1140.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1140.00		NIST Webbook
ripol	1369.00		NIST Webbook
ripol	1374.00		NIST Webbook
tb	457.28	K	Joback Method
tc	684.03	K	Joback Method
tf	310.27	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.63	J/mol×K	457.28	Joback Method
cpg	262.96	J/mol×K	495.07	Joback Method
cpg	281.10	J/mol×K	532.86	Joback Method
cpg	298.11	J/mol×K	570.66	Joback Method
cpg	314.04	J/mol×K	608.45	Joback Method
cpg	328.94	J/mol×K	646.24	Joback Method
cpg	342.87	J/mol×K	684.03	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	345.70	K	2.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4375148&Units=SI
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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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