1H-Indole, octahydro-3-methyl-

Other names: 3-Methyloctahydro-1H-indole
3-Methyl-octahydroindole
Skatole, perhydro-
Inchi: InChI=1S/C9H17N/c1-7-6-10-9-5-3-2-4-8(7)9/h7-10H,2-6H2,1H3
InchiKey: ZCJGZUQXRFHPQL-UHFFFAOYSA-N
Formula: C9H17N
SMILES: CC1CNC2CCCCC12
Mol. weight [g/mol]: 139.24
CAS: 37865-94-4

Physical Properties

Property code	Value	Unit	Source
gf	190.10	kJ/mol	Joback Method
hf	-84.50	kJ/mol	Joback Method
hfus	19.70	kJ/mol	Joback Method
hvap	42.42	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.785		Crippen Method
mcvol	125.930	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinpol	1217.00		NIST Webbook
rinpol	1235.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1415.00		NIST Webbook
tb	475.49	K	Joback Method
tc	698.44	K	Joback Method
tf	317.30	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.18	J/mol×K	475.49	Joback Method
cpg	309.76	J/mol×K	512.65	Joback Method

cpg	329.16	J/mol×K	549.81	Joback Method
cpg	347.41	J/mol×K	586.96	Joback Method
cpg	364.56	J/mol×K	624.12	Joback Method
cpg	380.66	J/mol×K	661.28	Joback Method
cpg	395.75	J/mol×K	698.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37865944&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

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