

n-Hexylmethamphetamine

Other names:	1-Hexanamine, N-methyl- Hexanamine, N-methyl- Hexylamine, N-methyl- Hexylmethamphetamine N-Methylhexylamine N-n-Hexylmethamphetamine methylhexylamine
Inchi:	InChI=1S/C7H17N/c1-3-4-5-6-7-8-2/h8H,3-7H2,1-2H3
InchiKey:	XJINZWNWPEQMMBV-UHFFFAOYSA-N
Formula:	C7H17N
SMILES:	CCCCCNC
Mol. weight [g/mol]:	115.22
CAS:	35161-70-7

Physical Properties

Property code	Value	Unit	Source
gf	97.45	kJ/mol	Joback Method
hf	-134.34	kJ/mol	Joback Method
hfus	18.98	kJ/mol	Joback Method
hvap	37.61	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.786		Crippen Method
mcvol	119.470	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
rinpol	871.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	871.00		NIST Webbook
tb	414.20	K	NIST Webbook
tc	592.00	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	221.31	K	Joback Method
vc	0.463	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.17	J/mol×K	409.73	Joback Method
cpg	250.74	J/mol×K	437.93	Joback Method
cpg	262.84	J/mol×K	466.14	Joback Method
cpg	274.48	J/mol×K	494.34	Joback Method
cpg	285.67	J/mol×K	522.55	Joback Method
cpg	296.42	J/mol×K	550.75	Joback Method
cpg	306.74	J/mol×K	578.95	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.57636e+01
Coeff. B	-3.98597e+03
Coeff. C	-5.65620e+01
Temperature range (K), min.	314.12
Temperature range (K), max.	437.92

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
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=C35161707&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvac:	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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/12-424-7/n-Hexylmethylamine.pdf>

Generated by Cheméo on 2024-04-26 08:20:32.443134108 +0000 UTC m=+16408881.363711425.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.