2-Hexanamine, 4-methyl-

Other names:	1,3-Dimethylamylamine
	1,3-Dimethylpentylamine
	2-Amino-4-methylhexane
	4-Methyl-2-hexanamine
	4-Methyl-2-hexylamine
	Forthan
	Forthane
	Methylhexaneamine
	NSC 1106
	Pentylamine, 1,3-dimethyl-
Inchi:	InChI=1S/C7H17N/c1-4-6(2)5-7(3)8/h6-7H,4-5,8H2,1-3H3
InchiKey:	YAHRDLICUYEDAU-UHFFFAOYSA-N
Formula:	C7H17N
SMILES:	CCC(C)CC(C)N
Mol. weight [g/mol]:	115.22
CAS:	105-41-9

Physical Properties

Property code	Value	Unit	Source
gf	69.63	kJ/mol	Joback Method
hf	-164.58	kJ/mol	Joback Method
hfus	12.04	kJ/mol	Joback Method
hvap	41.04	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.770		Crippen Method
mcvol	119.470	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
rinpol	1152.30		NIST Webbook
rinpol	1152.30		NIST Webbook
tb	431.21	K	Joback Method
tc	618.16	K	Joback Method
tf	221.91	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.79	J/mol×K	431.21	Joback Method
cpg	264.14	J/mol×K	462.37	Joback Method
cpg	276.91	J/mol×K	493.53	Joback Method
cpg	289.13	J/mol×K	524.68	Joback Method
cpg	300.81	J/mol×K	555.84	Joback Method
cpg	311.97	J/mol×K	587.00	Joback Method
cpg	322.62	J/mol×K	618.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43690e+01
Coeff. B	-3.55694e+03
Coeff. C	-5.39210e+01
Temperature range (K), min.	306.52
Temperature range (K), max.	446.63

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C105419&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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