2-Heptanamine, 6-methyl-

Other names:	1,5-Dimethylhexanamine
	1,5-Dimethylhexylamine
	2-Amino-6-Methylheptane
	2-Heptylamine, 6-methyl-
	2-Isooctylamine
	2-Methyl-6-aminoheptane
	2-Metil-6-amino-eptano
	6-Amino-2-methylheptane
	6-Methyl-2-heptylamine
	Amidrine
	Hexylamine, 1,5-dimethyl-
	Isoctaminum
	Octodrin
	SK&F-51
	SKF 51
	Vaporpac
	«alpha»,«epsilon»-Dimethylhexylamine
Inchi:	InChI=1S/C8H19N/c1-7(2)5-4-6-8(3)9/h7-8H,4-6,9H2,1-3H3
InchiKey:	QNIVIMYXGGFTAK-UHFFFAOYSA-N
Formula:	C8H19N
SMILES:	CC(C)CCCC(C)N
Mol. weight [g/mol]:	129.25
CAS:	543-82-8

Physical Properties

Property code	Value	Unit	Source
af	0.4691		Cheméo Relay (1.0)
gf	78.05	kJ/mol	Joback Method
hf	-211.06	kJ/mol	Cheméo Relay (1.0)
hfus	14.63	kJ/mol	Joback Method
hvap	47.42	kJ/mol	Cheméo Relay (1.0)
ie	8.51	eV	Cheméo Relay (1.0)
log10ws	-2.65		Cheméo Relay (1.0)
logp	2.160		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
rinpol	923.00		NIST Webbook

ripol	1132.00		NIST Webbook
ripol	1132.00		NIST Webbook
tb	428.20	K	NIST Webbook
tc	602.31	K	Cheméo Relay (1.0)
tf	218.12	K	Cheméo Relay (1.0)
vc	0.489	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.77	J/mol×K	454.09	Joback Method
cpg	307.18	J/mol×K	484.96	Joback Method
cpg	320.97	J/mol×K	515.83	Joback Method
cpg	334.15	J/mol×K	546.71	Joback Method
cpg	346.76	J/mol×K	577.58	Joback Method
cpg	358.79	J/mol×K	608.45	Joback Method
cpg	370.27	J/mol×K	639.32	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56600e+01
Coeff. B	-4.06362e+03
Coeff. C	-6.01760e+01
Temperature range (K), min.	298.15
Temperature range (K), max.	452.85

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C543828&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume