N,1-Dimethylhexylamine

Other names:	Hexylamine, N,1-dimethyl-
	Neosupranol
	Oenethyl
	Pacamine
	2-Heptanamine, N-methyl-
	2-Heptylmethylamine
	2-Methylaminoheptane
	Methyl(2-heptyl)amine
	NSC 27122
	Methylaminoheptane
Inchi:	InChI=1S/C8H19N/c1-4-5-6-7-8(2)9-3/h8-9H,4-7H2,1-3H3
InchiKey:	BGWFQRDYRSCOCO-UHFFFAOYSA-N
Formula:	C8H19N
SMILES:	CCCCCC(C)NC
Mol. weight [g/mol]:	129.24
CAS:	540-43-2

Physical Properties

Property code	Value	Unit	Source
gf	103.43	kJ/mol	Joback Method
hf	-160.26	kJ/mol	Joback Method
hfus	18.05	kJ/mol	Joback Method
hvap	39.45	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.175		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	990.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	992.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1130.00		NIST Webbook
ripol	1126.00		NIST Webbook
ripol	1147.00		NIST Webbook
ripol	1126.00		NIST Webbook
ripol	1130.00		NIST Webbook

tb	432.17	K	Joback Method
tc	604.23	K	Joback Method
tf	217.58	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.40	J/mol×K	432.17	Joback Method
cpg	293.41	J/mol×K	460.85	Joback Method
cpg	306.87	J/mol×K	489.52	Joback Method
cpg	319.80	J/mol×K	518.20	Joback Method
cpg	332.20	J/mol×K	546.88	Joback Method
cpg	344.10	J/mol×K	575.56	Joback Method
cpg	355.50	J/mol×K	604.23	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C540432&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume