Methyl(2-heptyl)amine

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]:	129.25

Physical Properties

Property code	Value	Unit	Source
af	0.4348		Cheméo Relay (1.0)
gf	103.43	kJ/mol	Joback Method
hf	-155.76	kJ/mol	Cheméo Relay (1.0)
hfus	18.05	kJ/mol	Joback Method
hvap	45.67	kJ/mol	Cheméo Relay (1.0)
ie	8.06	eV	Cheméo Relay (1.0)
log10ws	-1.34		Cheméo Relay (1.0)
logp	2.175		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	992.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	990.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1130.00		NIST Webbook
ripol	1126.00		NIST Webbook
ripol	1126.00		NIST Webbook
ripol	1147.00		NIST Webbook

ripol	1130.00		NIST Webbook
tb	426.96	K	Cheméo Relay (1.0)
tc	598.89	K	Cheméo Relay (1.0)
tf	237.70	K	Cheméo Relay (1.0)
vc	0.497	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C540432&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

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
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