1-Pentanamine, N-pentyl-

Other names:	DIPENTYLAMINE
	Di-n-amylamine
	Di-n-pentylamine
	Diamylamine
	N-pentyl-1-pentanamine
	N-pentylpentanamine
	PENTYL-PENTYLAMINE
	Pentylamine, pentyl-
	UN 2841
	pentanamine, N-pentyl-
Inchi:	InChI=1S/C10H23N/c1-3-5-7-9-11-10-8-6-4-2/h11H,3-10H2,1-2H3
InchiKey:	JACMPVXHEARCBO-UHFFFAOYSA-N
Formula:	C10H23N
SMILES:	CCCCCNCCCCC
Mol. weight [g/mol]:	157.30
CAS:	2050-92-2

Physical Properties

Property code	Value	Unit	Source
gf	122.71	kJ/mol	Joback Method
hf	-196.26	kJ/mol	Joback Method
hfus	26.75	kJ/mol	Joback Method
hvap	44.29	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.956		Crippen Method
mcvol	161.740	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
rinpol	1145.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1145.00		NIST Webbook
ripol	1300.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1295.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1302.00		NIST Webbook
tb	477.15 ± 0.00	K	NIST Webbook
tb	475.70	K	NIST Webbook

tb	476.15 ± 2.00	K	NIST Webbook
tb	478.15 ± 6.00	K	NIST Webbook
tb	475.65 ± 3.00	K	NIST Webbook
tc	644.75	K	Joback Method
tf	255.12	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.27	J/mol×K	589.29	Joback Method
cpg	439.38	J/mol×K	617.02	Joback Method
cpg	368.12	J/mol×K	478.37	Joback Method
cpg	383.54	J/mol×K	506.10	Joback Method
cpg	398.36	J/mol×K	533.83	Joback Method
cpg	412.60	J/mol×K	561.56	Joback Method
cpg	451.96	J/mol×K	644.75	Joback Method
hvapt	61.20	kJ/mol	298.15	The vaporization enthalpy and vapor pressure of S (+)-methamphetamine at T = 298.15 K by correlation gas chromatography
hvapt	51.20	kJ/mol	453.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.20	K	1.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.57313e+01
Coeff. B	-4.46940e+03
Coeff. C	-7.35200e+01
Temperature range (K), min.	362.92
Temperature range (K), max.	502.45

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1279.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2050922&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
The vaporization enthalpy and vapor pressure of S (+)-methamphetamine at T = 298.15 K by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2013.08.005
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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume