DIPENTYLAMINE

Other names:	1-Pentanamine, N-pentyl- Di-n-amylamine Di-n-pentylamine N-pentyl-1-pentanamine N-pentylpentanamine PENTYL-PENTYLAMINE Pentylamine, pentyl- UN 2841 diamylamine 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
af	0.5669		Cheméo Relay (1.0)
gf	122.71	kJ/mol	Joback Method
hf	-208.37	kJ/mol	Cheméo Relay (1.0)
hfus	26.75	kJ/mol	Joback Method
hvap	53.85	kJ/mol	Cheméo Relay (1.0)
ie	7.93	eV	Cheméo Relay (1.0)
log10ws	-2.65		Cheméo Relay (1.0)
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	1305.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1295.00		NIST Webbook
ripol	1300.00		NIST Webbook
ripol	1302.00		NIST Webbook

tb	475.70	K	NIST Webbook
tb	477.15 ± 0.00	K	NIST Webbook
tb	475.65 ± 3.00	K	NIST Webbook
tb	478.15 ± 6.00	K	NIST Webbook
tb	476.15 ± 2.00	K	NIST Webbook
tc	635.64	K	Cheméo Relay (1.0)
tf	244.40	K	Cheméo Relay (1.0)
vc	0.626	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	426.27	J/mol×K	589.29	Joback Method
cpg	439.38	J/mol×K	617.02	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2050922&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1279.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Cheméo Relay (1.0, beta):	

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume