Pentadecylamine

Other names:	1-Pentadecanamine
	1-Pentadecylamine
	Pentadecane, 1-amino-
	n-Pentadecylamine
Inchi:	InChI=1S/C15H33N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16/h2-16H2,1H3
InchiKey:	JPZYXGPCHFZBHO-UHFFFAOYSA-N
Formula:	C15H33N
SMILES:	CCCCCCCCCCCCCCCN
Mol. weight [g/mol]:	227.43
CAS:	2570-26-5

Physical Properties

Property code	Value	Unit	Source
gf	141.87	kJ/mol	Joback Method
hf	-319.14	kJ/mol	Joback Method
hfus	39.80	kJ/mol	Joback Method
hvap	88.10 ± 0.30	kJ/mol	NIST Webbook
log10ws	-5.54		Crippen Method
logp	5.036		Crippen Method
mcvol	232.190	ml/mol	McGowan Method
pc	1478.15	kPa	Joback Method
rinpol	2025.00		NIST Webbook
tb	580.00	K	NIST Webbook
tb	572.65 ± 5.00	K	NIST Webbook
tb	580.80	K	NIST Webbook
tc	784.02	K	Joback Method
tf	313.15 ± 2.00	K	NIST Webbook
tf	310.15 ± 1.00	K	NIST Webbook
tf	306.65 ± 2.00	K	NIST Webbook
tf	309.65 ± 0.50	K	NIST Webbook
tf	309.65 ± 0.50	K	NIST Webbook
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.05	J/mol×K	615.13	Joback Method
cpg	656.38	J/mol×K	643.28	Joback Method
cpg	673.92	J/mol×K	671.43	Joback Method
cpg	690.71	J/mol×K	699.57	Joback Method
cpg	706.77	J/mol×K	727.72	Joback Method
cpg	722.12	J/mol×K	755.87	Joback Method
cpg	736.79	J/mol×K	784.02	Joback Method
hvapt	75.50	kJ/mol	499.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61828e+01
Coeff. B	-5.51276e+03
Coeff. C	-1.04100e+02
Temperature range (K), min.	450.92
Temperature range (K), max.	611.19

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2570265&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume