1-Undecanamine

Other names:	1-AMINOUNDECANE
	1-Undecylamine
	HENDECYLAMINE
	Undecylamine
	n-Undecylamine
Inchi:	InChI=1S/C11H25N/c1-2-3-4-5-6-7-8-9-10-11-12/h2-12H2,1H3
InchiKey:	QFKMMXYLAPZKIB-UHFFFAOYSA-N
Formula:	C11H25N
SMILES:	CCCCCCCCCCCN
Mol. weight [g/mol]:	171.32
CAS:	7307-55-3

Physical Properties

Property code	Value	Unit	Source
gf	108.19	kJ/mol	Joback Method
hf	-236.58	kJ/mol	Joback Method
hfus	29.44	kJ/mol	Joback Method
hvap	50.72	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.476		Crippen Method
mcvol	175.830	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
rinpol	1330.00		NIST Webbook
rinpol	1330.00		NIST Webbook
ripol	1625.00		NIST Webbook
ripol	1623.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1623.00		NIST Webbook
tb	515.00	K	NIST Webbook
tb	513.20	K	NIST Webbook
tb	515.20	K	NIST Webbook
tc	696.54	K	Joback Method
tf	288.15 ± 1.00	K	NIST Webbook
tf	288.65 ± 2.00	K	NIST Webbook
tf	288.15 ± 1.00	K	NIST Webbook

vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.29	J/mol×K	523.61	Joback Method
cpg	446.41	J/mol×K	552.43	Joback Method
cpg	461.86	J/mol×K	581.25	Joback Method
cpg	476.67	J/mol×K	610.07	Joback Method
cpg	490.84	J/mol×K	638.90	Joback Method
cpg	504.40	J/mol×K	667.72	Joback Method
cpg	517.38	J/mol×K	696.54	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58459e+01
Coeff. B	-4.81608e+03
Coeff. C	-8.42500e+01
Temperature range (K), min.	393.80
Temperature range (K), max.	541.42

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.04557e+02
Coeff. B	-1.13349e+04
Coeff. C	-1.27040e+01
Coeff. D	5.28499e-06
Temperature range (K), min.	428.15
Temperature range (K), max.	527.15

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1280.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7307553&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1280
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

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
pvap:	Vapor 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