TRIDECYLAMINE

Other names:	1-Aminotridecane
	Monotridecylamine
	n-Tridecylamine
Inchi:	InChI=1S/C13H29N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14/h2-14H2,1H3
InchiKey:	ABVVEAHYODGCLZ-UHFFFAOYSA-N
Formula:	C13H29N
SMILES:	CCCCCCCCCCCCCN
Mol. weight [g/mol]:	199.38
CAS:	2869-34-3

Physical Properties

Property code	Value	Unit	Source
af	0.7260		Cheméo Relay (1.0)
gf	125.03	kJ/mol	Joback Method
hf	-309.77	kJ/mol	Cheméo Relay (1.0)
hfus	34.62	kJ/mol	Joback Method
hvap	77.62	kJ/mol	Cheméo Relay (1.0)
ie	8.76	eV	Cheméo Relay (1.0)
log10ws	-5.50		Cheméo Relay (1.0)
logp	4.256		Crippen Method
mcvol	204.010	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
tb	538.20	K	NIST Webbook
tb	548.00	K	NIST Webbook
tb	703.15 ± 4.00	K	NIST Webbook
tb	538.15 ± 6.00	K	NIST Webbook
tc	715.97	K	Cheméo Relay (1.0)
tf	300.15 ± 2.00	K	NIST Webbook
tf	300.65 ± 2.00	K	NIST Webbook
vc	0.806	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	531.05	J/mol×K	569.37	Joback Method
cpg	548.39	J/mol×K	597.78	Joback Method
cpg	565.01	J/mol×K	626.19	Joback Method
cpg	580.92	J/mol×K	654.60	Joback Method
cpg	596.14	J/mol×K	683.02	Joback Method
cpg	610.71	J/mol×K	711.43	Joback Method
cpg	624.63	J/mol×K	739.84	Joback Method
hvapt	76.80	kJ/mol	652.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61780e+01
Coeff. B	-5.23738e+03
Coeff. C	-9.49260e+01
Temperature range (K), min.	424.52
Temperature range (K), max.	576.90

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2869343&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

Cheméo Relay (1.0):

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