

1-Dodecanamine, N,N-diethyl-

Other names:	Diethyldodecylamine Dodecylamine, N,N-diethyl- N,N-Diethyl dodecyl amine N-Dodecyldiethylamine
Inchi:	InChI=1S/C16H35N/c1-4-7-8-9-10-11-12-13-14-15-16-17(5-2)6-3/h4-16H2,1-3H3
InchiKey:	IOKYPACLTOWHCM-UHFFFAOYSA-N
Formula:	C16H35N
SMILES:	CCCCCCCCCCCCCN(CC)CC
Mol. weight [g/mol]:	241.46
CAS:	4271-27-6

Physical Properties

Property code	Value	Unit	Source
gf	194.62	kJ/mol	Joback Method
hf	-306.04	kJ/mol	Joback Method
hfus	40.22	kJ/mol	Joback Method
hvap	53.25	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	5.249		Crippen Method
mcvol	246.280	ml/mol	McGowan Method
pc	1316.56	kPa	Joback Method
rinpol	1642.00		NIST Webbook
rinpol	1642.00		NIST Webbook
tb	577.92	K	Joback Method
tc	735.96	K	Joback Method
tf	302.55	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.37	J/mol×K	577.92	Joback Method
cpg	670.88	J/mol×K	604.26	Joback Method
cpg	689.61	J/mol×K	630.60	Joback Method

cpg	707.58	J/mol×K	656.94	Joback Method
cpg	724.81	J/mol×K	683.28	Joback Method
cpg	741.32	J/mol×K	709.62	Joback Method
cpg	757.14	J/mol×K	735.96	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51205e+01
Coeff. B	-4.86561e+03
Coeff. C	-9.40920e+01
Temperature range (K), min.	422.12
Temperature range (K), max.	590.13

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C4271276&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

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

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