

Dimethyl palmitamine

Other names:	1-Hexadecanamine, N,N-dimethyl- Adma 16 amine Armeen DM 16D Cetyldimethylamine Dimethyl-1-hexadecanamine Dimethyl-n-hexadecylamine Dimethylcetylamine Dimethylhexadecylamine Dimethylpalmitylamine Farmin DM 60 Genamin 16R302D Hexadecylamine, N,N-dimethyl- Hexadecyldimethylamine IPL 67 N,N-Dimethyl-1-hexadecanamine N,N-Dimethyl-n-hexadecylamine N,N-Dimethylcetylamine N,N-Dimethylhexadecylamine N,N-Dimethylpalmitylamine N-Hexadecyldimethylamine NSC 404177 Palmityl Dimethyl Amine
Inchi:	InChI=1S/C18H39N/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(2)3/h4-18H2,1-3H3
InchiKey:	NHLUVTZJQOJKCC-UHFFFAOYSA-N
Formula:	C18H39N
SMILES:	CCCCCCCCCCCCCCCCN(C)C
Mol. weight [g/mol]:	269.51
CAS:	112-69-6

Physical Properties

Property code	Value	Unit	Source
gf	211.46	kJ/mol	Joback Method
hf	-347.32	kJ/mol	Joback Method
hfus	45.40	kJ/mol	Joback Method
hvap	57.70	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method

logp	6.029		Crippen Method
mvol	274.460	ml/mol	McGowan Method
pc	1150.65	kPa	Joback Method
rinpol	1894.00		NIST Webbook
tb	623.68	K	Joback Method
tc	782.28	K	Joback Method
tf	285.15 ± 2.00	K	NIST Webbook
vc	1.062	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.90	J/mol×K	623.68	Joback Method
cpg	785.25	J/mol×K	650.11	Joback Method
cpg	804.77	J/mol×K	676.55	Joback Method
cpg	823.47	J/mol×K	702.98	Joback Method
cpg	841.39	J/mol×K	729.41	Joback Method
cpg	858.55	J/mol×K	755.84	Joback Method
cpg	874.99	J/mol×K	782.28	Joback Method
hvapt	84.80	kJ/mol	298.00	Evaluation of the Vaporization Enthalpies and Liquid Vapor Pressures of (R)-Deprenyl, (S)-Benzphetamine, Alverine, and a Series of Aliphatic Tertiary Amines by Correlation Gas Chromatography at T/K = 298.15
hvapt	67.30	kJ/mol	577.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.73201e+01
Coeff. B	-6.05836e+03

Coeff. C	-1.08826e+02
Temperature range (K), min.	464.52
Temperature range (K), max.	613.33

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112696&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Evaluation of the Vaporization Enthalpies and Liquid Vapor Pressures of the Method; (S)-Benzphetamine, Alverine, and a Series of Aliphatic Tertiary Amines by Correlation Gas Chromatography at T/K = 298.15:	https://www.doi.org/10.1021/je500358r
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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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