

Dodecylamine, N,N-di(allyl)-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C18H35N/c1-4-7-8-9-10-11-12-13-14-15-18-19(16-5-2)17-6-3/h5-6H,2-4,7-18H

CMQARNDWULTILC-UHFFFAOYSA-N

C18H35N

C=CCN(CC=C)CCCCCCCCCCCC

265.48

Physical Properties

Property code	Value	Unit	Source
gf	387.14	kJ/mol	Joback Method
hf	-96.46	kJ/mol	Joback Method
hfus	42.84	kJ/mol	Joback Method
hvap	56.36	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.581		Crippen Method
mcvol	265.860	ml/mol	McGowan Method
pc	1219.14	kPa	Joback Method
rinpol	2265.00		NIST Webbook
rinpol	2265.00		NIST Webbook
tb	617.04	K	Joback Method
tc	779.06	K	Joback Method
tf	321.57	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.70	J/mol×K	617.04	Joback Method
cpg	739.19	J/mol×K	644.04	Joback Method
cpg	757.82	J/mol×K	671.05	Joback Method
cpg	775.63	J/mol×K	698.05	Joback Method
cpg	792.66	J/mol×K	725.05	Joback Method
cpg	808.94	J/mol×K	752.06	Joback Method
cpg	824.51	J/mol×K	779.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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