

Hexadecylamine, N-allyl-

Inchi:	InChI=1S/C19H39N/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-19-20-18-4-2/h4,20H,2-3,5
InchiKey:	BGMODKVMRWSBLQ-UHFFFAOYSA-N
Formula:	C19H39N
SMILES:	C=CCNCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	281.52

Physical Properties

Property code	Value	Unit	Source
gf	286.33	kJ/mol	Joback Method
hf	-256.59	kJ/mol	Joback Method
hfus	48.79	kJ/mol	Joback Method
hvap	63.65	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	6.243		Crippen Method
mvol	284.250	ml/mol	McGowan Method
pc	1120.80	kPa	Joback Method
rinpol	2698.00		NIST Webbook
tb	680.97	K	Joback Method
tc	846.77	K	Joback Method
tf	354.79	K	Joback Method
vc	1.115	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.69	J/mol×K	680.97	Joback Method
cpg	846.42	J/mol×K	708.60	Joback Method
cpg	865.29	J/mol×K	736.24	Joback Method
cpg	883.33	J/mol×K	763.87	Joback Method
cpg	900.57	J/mol×K	791.50	Joback Method
cpg	917.04	J/mol×K	819.14	Joback Method
cpg	932.76	J/mol×K	846.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416168&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

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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