Octadecylamine, N-allyl-

Inchi: InChI=1S/C21H43N/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21-22-20-4-2/h4,22H
InchiKey: NZDBTPVECFIJKC-UHFFFAOYSA-N
Formula: C21H43N
SMILES: C=CCNCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 309.57

Physical Properties

Property code	Value	Unit	Source
gf	303.17	kJ/mol	Joback Method
hf	-297.87	kJ/mol	Joback Method
hfus	53.96	kJ/mol	Joback Method
hvap	68.11	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	7.024		Crippen Method
mcvol	312.430	ml/mol	McGowan Method
pc	989.51	kPa	Joback Method
rinpol	1088.00		NIST Webbook
tb	726.73	K	Joback Method
tc	895.81	K	Joback Method
tf	377.33	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	946.83	J/mol×K	726.73	Joback Method
cpg	967.42	J/mol×K	754.91	Joback Method
cpg	987.08	J/mol×K	783.09	Joback Method
cpg	1005.85	J/mol×K	811.27	Joback Method
cpg	1023.75	J/mol×K	839.45	Joback Method
cpg	1040.83	J/mol×K	867.63	Joback Method
cpg	1057.13	J/mol×K	895.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416169&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume