

Octylamine, N-allyl-

Inchi:	InChI=1S/C11H23N/c1-3-5-6-7-8-9-11-12-10-4-2/h4,12H,2-3,5-11H2,1H3
InchiKey:	SHLPFDHXCIUODM-UHFFFAOYSA-N
Formula:	C11H23N
SMILES:	C=CCNCCCCCCCC
Mol. weight [g/mol]:	169.31

Physical Properties

Property code	Value	Unit	Source
gf	218.97	kJ/mol	Joback Method
hf	-91.47	kJ/mol	Joback Method
hfus	28.07	kJ/mol	Joback Method
hvap	45.85	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.123		Crippen Method
mcvol	171.530	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	1306.00		NIST Webbook
rinpol	1306.00		NIST Webbook
tb	497.93	K	Joback Method
tc	666.24	K	Joback Method
tf	264.63	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.94	J/mol×K	497.93	Joback Method
cpg	412.64	J/mol×K	525.98	Joback Method
cpg	427.68	J/mol×K	554.03	Joback Method
cpg	442.10	J/mol×K	582.08	Joback Method
cpg	455.90	J/mol×K	610.14	Joback Method
cpg	469.12	J/mol×K	638.19	Joback Method
cpg	481.76	J/mol×K	666.24	Joback Method

Sources

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=U416163&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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