

ALLYLCYCLOHEXYLAMINE

Other names:	Allylcyclohexylamine N-allylcyclohexylamine
Inchi:	InChI=1S/C9H17N/c1-2-8-10-9-6-4-3-5-7-9/h2,9-10H,1,3-8H2
InchiKey:	SQGBZKZDUMBTIJ-UHFFFAOYSA-N
Formula:	C9H17N
SMILES:	C=CCNC1CCCCC1
Mol. weight [g/mol]:	139.24

Physical Properties

Property code	Value	Unit	Source
hfus	14.72	kJ/mol	Joback Method
hvap	52.60	kJ/mol	Cheméo Relay (1.0)
ie	8.26	eV	Cheméo Relay (1.0)
logp	2.095		Crippen Method
mcvol	132.490	ml/mol	McGowan Method
tb	463.72	K	Cheméo Relay (1.0)
tf	240.81	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.54	J/mol×K	471.72	Joback Method
cpg	308.69	J/mol×K	506.07	Joback Method
cpg	325.85	J/mol×K	540.43	Joback Method
cpg	342.07	J/mol×K	574.78	Joback Method
cpg	357.37	J/mol×K	609.14	Joback Method
cpg	371.78	J/mol×K	643.49	Joback Method
cpg	385.35	J/mol×K	677.85	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	338.70	K	1.60	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6628008&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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