

Allyldiethylamine

Other names:	2-Propen-1-amine, N,N-diethyl- N,N-Diethylallylamine N-Allyldiethylamine
Inchi:	InChI=1S/C7H15N/c1-4-7-8(5-2)6-3/h4H,1,5-7H2,2-3H3
InchiKey:	JWAJUTZQGZBKFS-UHFFFAOYSA-N
Formula:	C7H15N
SMILES:	C=CCN(CC)CC
Mol. weight [g/mol]:	113.20
CAS:	5666-17-1

Physical Properties

Property code	Value	Unit	Source
gf	206.68	kJ/mol	Joback Method
hf	5.15	kJ/mol	Joback Method
hfus	15.63	kJ/mol	Joback Method
hvap	32.55	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	1.514		Crippen Method
mcvol	115.170	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
rinpola	751.00		NIST Webbook
rinpola	751.00		NIST Webbook
tb	336.50 ± 0.50	K	NIST Webbook
tc	534.54	K	Joback Method
tf	199.36	K	Joback Method
vc	0.426	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.15	J/mol×K	368.68	Joback Method
cpg	219.64	J/mol×K	396.32	Joback Method
cpg	231.60	J/mol×K	423.97	Joback Method
cpg	243.06	J/mol×K	451.61	Joback Method

cpg	254.03	J/mol×K	479.25	Joback Method
cpg	264.53	J/mol×K	506.90	Joback Method
cpg	274.56	J/mol×K	534.54	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.15534e+01
Coeff. B	-2.41655e+03
Coeff. C	-3.46970e+01
Temperature range (K), min.	249.20
Temperature range (K), max.	421.84

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5666171&Units=SI

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

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

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