N-Allylaniline

Other names: Benzenamine, N-2-propenyl-
Inchi: InChI=1S/C9H11N/c1-2-8-10-9-6-4-3-5-7-9/h2-7,10H,1,8H2
InchiKey: LQFLWKPCQITJIH-UHFFFAOYSA-N
Formula: C9H11N
SMILES: C=CCNc1ccccc1
Mol. weight [g/mol]: 133.19
CAS: 589-09-3

Physical Properties

Property code	Value	Unit	Source
gf	314.54	kJ/mol	Joback Method
hf	186.34	kJ/mol	Joback Method
hfus	16.93	kJ/mol	Joback Method
hvap	43.67	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	2.284		Crippen Method
mcvol	119.590	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	492.20	K	NIST Webbook
tc	692.92	K	Joback Method
tf	268.51	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.00	J/mol×K	478.85	Joback Method
cpg	256.63	J/mol×K	514.53	Joback Method
cpg	269.40	J/mol×K	550.21	Joback Method
cpg	281.34	J/mol×K	585.88	Joback Method
cpg	292.51	J/mol×K	621.56	Joback Method
cpg	302.93	J/mol×K	657.24	Joback Method
cpg	312.66	J/mol×K	692.92	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	491.20	K	98.10	NIST Webbook

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=C589093&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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