

allyl-N-methylaniline

Inchi:	InChI=1S/C10H13N/c1-3-9-11(2)10-7-5-4-6-8-10/h3-8H,1,9H2,2H3
InchiKey:	WJYIMFNLIJXFMX-UHFFFAOYSA-N
Formula:	C10H13N
SMILES:	C=CCN(C)c1ccccc1
Mol. weight [g/mol]:	147.22

Physical Properties

Property code	Value	Unit	Source
gf	344.35	kJ/mol	Joback Method
hf	179.76	kJ/mol	Joback Method
hfus	17.44	kJ/mol	Joback Method
hvap	41.50	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	2.309		Crippen Method
mcvol	133.680	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rmpol	1214.00		NIST Webbook
tb	464.00	K	Joback Method
tc	670.40	K	Joback Method
tf	259.59	K	Joback Method
vc	0.486	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.29	J/mol×K	464.00	Joback Method
cpg	286.71	J/mol×K	498.40	Joback Method
cpg	301.18	J/mol×K	532.80	Joback Method
cpg	314.73	J/mol×K	567.20	Joback Method
cpg	327.42	J/mol×K	601.60	Joback Method
cpg	339.28	J/mol×K	636.00	Joback Method
cpg	350.37	J/mol×K	670.40	Joback Method

Sources

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=R390715&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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