

4-H2NC6H4C(CH3)=CH2

Inchi:	InChI=1S/C9H11N/c1-7(2)8-3-5-9(10)6-4-8/h3-6H,1,10H2,2H3
InchiKey:	IZSICESBWDKSCB-UHFFFAOYSA-N
Formula:	C9H11N
SMILES:	C=C(C)c1ccc(N)cc1
Mol. weight [g/mol]:	133.19
CAS:	1962-08-9

Physical Properties

Property code	Value	Unit	Source
affp	929.80	kJ/mol	NIST Webbook
basg	903.30	kJ/mol	NIST Webbook
gf	273.42	kJ/mol	Joback Method
hf	145.40	kJ/mol	Joback Method
hfus	15.32	kJ/mol	Joback Method
hvap	48.62	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.302		Crippen Method
mcvol	119.590	ml/mol	McGowan Method
pc	3620.24	kPa	Joback Method
tb	506.07	K	Joback Method
tc	736.19	K	Joback Method
tf	297.67	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.38	J/mol×K	506.07	Joback Method
cpg	266.55	J/mol×K	544.42	Joback Method
cpg	278.87	J/mol×K	582.78	Joback Method
cpg	290.36	J/mol×K	621.13	Joback Method
cpg	301.09	J/mol×K	659.48	Joback Method
cpg	311.08	J/mol×K	697.83	Joback Method
cpg	320.39	J/mol×K	736.19	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=C1962089&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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