2-Imidazoline, 2-(p-aminophenyl)-

Inchi: InChI=1S/C9H11N3/c10-8-3-1-7(2-4-8)9-11-5-6-12-9/h1-4H,5-6,10H2,(H,11,12)
InchiKey: HSJPRHDSBNINIJ-UHFFFAOYSA-N
Formula: C9H11N3
SMILES: Nc1ccc(C2=NCCN2)cc1
Mol. weight [g/mol]: 161.20
CAS: 61033-71-4

Physical Properties

Property code	Value	Unit	Source
gf	463.21	kJ/mol	Joback Method
hf	265.67	kJ/mol	Joback Method
hfus	26.34	kJ/mol	Joback Method
hvap	63.69	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	0.619		Crippen Method
mcvol	128.690	ml/mol	McGowan Method
pc	4762.81	kPa	Joback Method
tb	635.85	K	Joback Method
tc	907.68	K	Joback Method
tf	518.38	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.89	J/mol×K	635.85	Joback Method
cpg	351.46	J/mol×K	681.15	Joback Method
cpg	365.74	J/mol×K	726.46	Joback Method
cpg	378.74	J/mol×K	771.76	Joback Method
cpg	390.52	J/mol×K	817.07	Joback Method
cpg	401.09	J/mol×K	862.37	Joback Method
cpg	410.50	J/mol×K	907.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61033714&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume