Acetylene, 1-(2-aminophenyl)-2-phenyl-

Inchi: InChI=1S/C14H11N/c15-14-9-5-4-8-13(14)11-10-12-6-2-1-3-7-12/h1-9H,15H2
InchiKey: BZDTZZOSIAUOBS-UHFFFAOYSA-N
Formula: C14H11N
SMILES: Nc1ccccc1C#Cc1ccccc1
Mol. weight [g/mol]: 193.24

Physical Properties

Property code	Value	Unit	Source
gf	551.44	kJ/mol	Joback Method
hf	435.39	kJ/mol	Joback Method
hfus	28.03	kJ/mol	Joback Method
hvap	64.77	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.669		Crippen Method
mcvol	161.980	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	1474.00		NIST Webbook
rinpol	1474.00		NIST Webbook
tb	659.59	K	Joback Method
tc	938.38	K	Joback Method
tf	502.26	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.60	J/mol×K	659.59	Joback Method
cpg	406.11	J/mol×K	706.06	Joback Method
cpg	420.24	J/mol×K	752.52	Joback Method
cpg	433.08	J/mol×K	798.99	Joback Method
cpg	444.74	J/mol×K	845.45	Joback Method
cpg	455.33	J/mol×K	891.92	Joback Method
cpg	464.94	J/mol×K	938.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380734&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume