m-Aminophenylacetylene

Other names:	Benzenamine, 3-ethynyl-
	3-ethynylaniline
Inchi:	InChI=1S/C8H7N/c1-2-7-4-3-5-8(9)6-7/h1,3-6H,9H2
InchiKey:	NNKQLUVBPJEUOR-UHFFFAOYSA-N
Formula:	C8H7N
SMILES:	C#Cc1cccc(N)c1
Mol. weight [g/mol]:	117.15
CAS:	54060-30-9

Physical Properties

Property code	Value	Unit	Source
gf	408.78	kJ/mol	Joback Method
hf	342.30	kJ/mol	Joback Method
hfus	18.30	kJ/mol	Joback Method
hvap	46.84	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.250		Crippen Method
mcvol	101.200	ml/mol	McGowan Method
pc	4659.34	kPa	Joback Method
tb	476.75	K	Joback Method
tc	719.01	K	Joback Method
tf	349.09	K	Joback Method
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.23	J/mol×K	476.75	Joback Method
cpg	207.96	J/mol×K	517.13	Joback Method
cpg	217.90	J/mol×K	557.50	Joback Method
cpg	227.12	J/mol×K	597.88	Joback Method
cpg	235.65	J/mol×K	638.26	Joback Method
cpg	243.53	J/mol×K	678.63	Joback Method
cpg	250.82	J/mol×K	719.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54060309&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