4-Aminothiophenol

Other names:	Benzenethiol, p-amino-
	p-Aminobenzenethiol
	p-Aminophenylmercaptan
	p-Aminothiophenol
	p-Mercaptoaniline
	4-Aminobenzenethiol
	4-Mercaptoaniline
	Benzenethiol, 4-amino-
Inchi:	InChI=1S/C6H7NS/c7-5-1-3-6(8)4-2-5/h1-4,8H,7H2
InchiKey:	WCDSVWRUXWCYFN-UHFFFAOYSA-N
Formula:	C6H7NS
SMILES:	Nc1ccc(S)cc1
Mol. weight [g/mol]:	125.19
CAS:	1193-02-8

Physical Properties

Property code	Value	Unit	Source
gf	198.26	kJ/mol	Joback Method
hf	130.16	kJ/mol	Joback Method
hfus	14.19	kJ/mol	Joback Method
hvap	49.27	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.558		Crippen Method
mcvol	97.970	ml/mol	McGowan Method
pc	5430.51	kPa	Joback Method
tb	503.73	K	Joback Method
tc	761.14	K	Joback Method
tf	319.00	K	NIST Webbook
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.97	J/mol×K	503.73	Joback Method

cpg	199.24	J/mol×K	546.63	Joback Method
cpg	208.76	J/mol×K	589.53	Joback Method
cpg	217.55	J/mol×K	632.44	Joback Method
cpg	225.66	J/mol×K	675.34	Joback Method
cpg	233.12	J/mol×K	718.24	Joback Method
cpg	239.97	J/mol×K	761.14	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	415.70	K	2.10	NIST Webbook
tbrp	415.00	K	2.00	NIST Webbook

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=C1193028&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume