

3-AMINOTHIOPHENOL

Other names:	Benzenethiol, 3-amino- 3-Aminothiophenol
Inchi:	InChI=1S/C6H7NS/c7-5-2-1-3-6(8)4-5/h1-4,8H,7H2
InchiKey:	KFFUEVDMVNIOHA-UHFFFAOYSA-N
Formula:	C6H7NS
SMILES:	Nc1cccc(S)c1
Mol. weight [g/mol]:	125.20

Physical Properties

Property code	Value	Unit	Source
af	0.4411		Cheméo Relay (1.0)
gf	198.26	kJ/mol	Joback Method
hf	114.45	kJ/mol	Cheméo Relay (1.0)
hfus	14.19	kJ/mol	Joback Method
hvap	71.22	kJ/mol	Cheméo Relay (1.0)
ie	7.68	eV	Cheméo Relay (1.0)
log10ws	-1.64		Cheméo Relay (1.0)
logp	1.558		Crippen Method
mcvol	97.970	ml/mol	McGowan Method
pc	5430.51	kPa	Joback Method
tb	537.96	K	Cheméo Relay (1.0)
tc	810.72	K	Cheméo Relay (1.0)
tf	302.04	K	Cheméo Relay (1.0)
vc	0.318	m3/kmol	Cheméo Relay (1.0)

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	458.20	K	2.10	NIST Webbook
tbrp	458.00 ± 5.00	K	2.10	NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C22948023&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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