Benzenethiol, 2-amino-

Other names:	o-Mercaptoaniline
	Benzenethiol, o-amino-
	o-Aminobenzenethiol
	o-Aminothiophenol
	1-Amino-2-mercaptobenzene
	2-Aminobenzenethiol
	2-Aminothiophenol
	2-Mercaptaniline
	2-Mercaptoaniline
	o-Aminophenyl mercaptan
	USAF EK-4376
	2-Aminophenyl mercaptan
	2-Amino-1-mercaptobenzene
Inchi:	InChI=1S/C6H7NS/c7-5-3-1-2-4-6(5)8/h1-4,8H,7H2
InchiKey:	VRVRGVPWCUEOGV-UHFFFAOYSA-N
Formula:	C6H7NS
SMILES:	Nc1ccccc1S
Mol. weight [g/mol]:	125.19
CAS:	137-07-5

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
ie	8.00	eV	NIST Webbook
ie	7.60	eV	NIST Webbook
log10ws	-1.62		Crippen Method
logp	1.558		Crippen Method
mcvol	97.970	ml/mol	McGowan Method
pc	5430.51	kPa	Joback Method
tb	507.20	K	NIST Webbook
tb	507.00	K	NIST Webbook
tc	761.14	K	Joback Method
tf	299.00	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	368.50 ± 1.50	K	0.50	NIST Webbook
tbrp	399.00 ± 1.00	K	0.80	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C137075&Units=SI

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
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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