4-(METHYLMERCAPTO)ANILINE

Other names: (4-(Methylthio)phenyl)amine
4-(Methylthio)aniline
4-(Methylthio)benzenamine
4-Aminothioanisole
Aniline, p-(methylthio)-
Benzenamine, 4-(methylthio)-
NSC 75842
p-(Methylthio)aniline
p-Aminophenyl methyl sulfide
p-Aminothioanisole
p-Thioanisidine
p-Thiomethoxyaniline

Inchi: InChI=1S/C7H9NS/c1-9-7-4-2-6(8)3-5-7/h2-5H,8H2,1H3

InchiKey: YKFROQCFVXOUPW-UHFFFAOYSA-N

Formula: C7H9NS

SMILES: CSc1ccc(N)cc1

Mol. weight [g/mol]: 139.22

Physical Properties

Property code	Value	Unit	Source
af	0.4413		Cheméo Relay (1.0)
hf	85.41	kJ/mol	Cheméo Relay (1.0)
hfus	16.86	kJ/mol	Joback Method
hvap	69.92	kJ/mol	Cheméo Relay (1.0)
ie	7.60	eV	NIST Webbook
ie	7.60 ± 0.01	eV	NIST Webbook
log10ws	-1.74		Cheméo Relay (1.0)
logp	1.991		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
pc	4444.44	kPa	Joback Method
tb	545.70	K	NIST Webbook
tb	545.50 ± 0.50	K	NIST Webbook
tc	759.17	K	Cheméo Relay (1.0)
tf	307.98	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.94	J/mol×K	532.53	Joback Method
cpg	243.64	J/mol×K	574.43	Joback Method
cpg	254.54	J/mol×K	616.33	Joback Method
cpg	264.66	J/mol×K	658.23	Joback Method
cpg	274.04	J/mol×K	700.13	Joback Method
cpg	282.69	J/mol×K	742.02	Joback Method
cpg	290.64	J/mol×K	783.92	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.20	K	2.00	NIST Webbook
tbrp	412.00	K	2.00	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C104961&Units=SI

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

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