Benzene, 1-methyl-4-(methylthio)-

Other names:	Sulfide, methyl p-tolyl
	p-(Methylthio)toluene
	p-Cresyl methyl sulfide
	p-Tolyl methyl sulfide
	Methyl p-cresyl sulfide
	Methyl p-tolyl sulfide
	4-(Methylthio)toluene
	p-Methylphenyl methyl sulfide
	4-Methyl-(1-thiaethyl)benzene
	p-Thiocresol, S-methyl-
	Methyl p-tolyl sulphide
	NSC 6256
	1-Methyl-4-(methylsulfanyl)benzene
Inchi:	InChI=1S/C8H10S/c1-7-3-5-8(9-2)6-4-7/h3-6H,1-2H3
InchiKey:	VHILIAIEEYLJNA-UHFFFAOYSA-N
Formula:	C8H10S
SMILES:	CSc1ccc(C)cc1
Mol. weight [g/mol]:	138.23
CAS:	623-13-2

Physical Properties

Property code	Value	Unit	Source
gf	152.38	kJ/mol	Joback Method
hf	58.48	kJ/mol	Joback Method
hfus	14.26	kJ/mol	Joback Method
hvap	43.16	kJ/mol	Joback Method
ie	7.90 ± 0.05	eV	NIST Webbook
ie	7.87	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
log10ws	-2.69		Crippen Method
logp	2.717		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
rinpol	1214.40		NIST Webbook
tb	482.88	K	Joback Method
tc	718.95	K	Joback Method
tf	253.26	K	Joback Method

vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.13	J/mol×K	482.88	Joback Method
cpg	235.96	J/mol×K	522.23	Joback Method
cpg	248.02	J/mol×K	561.57	Joback Method
cpg	259.35	J/mol×K	600.92	Joback Method
cpg	269.95	J/mol×K	640.26	Joback Method
cpg	279.85	J/mol×K	679.61	Joback Method
cpg	289.08	J/mol×K	718.95	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	326.20	K	0.10	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C623132&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume