Benzene, 1-methyl-2-(methylthio)-

Other names:	Sulfide, methyl o-tolyl
	o-Cresyl methyl sulfide
	Methyl o-tolyl sulfide
	2-Methyl-(1-thiaethyl)benzene
	2-Methylbenzenethiol, S-methyl-
	methyl 2-methylphenyl sulfide
	1-Methyl-2-(methylsulfanyl)benzene
Inchi:	InChI=1S/C8H10S/c1-7-5-3-4-6-8(7)9-2/h3-6H,1-2H3
InchiKey:	BHWJMPDCCDMCKC-UHFFFAOYSA-N
Formula:	C8H10S
SMILES:	CSc1ccccc1C
Mol. weight [g/mol]:	138.23
CAS:	14092-00-3

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
log10ws	-2.69		Crippen Method
logp	2.717		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
rinpol	1210.10		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1209.00		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

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14092003&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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