

Benzene, 1-methyl-3-(methylthio)-

Other names:	Sulfide, methyl m-tolyl m-Methylthioanisole Methyl m-tolyl sulfide 3-Methylthiotoluene 3-Methylbenzenethiol, S-methyl- 1-Methyl-3-(methylsulfanyl)benzene
Inchi:	InChI=1S/C8H10S/c1-7-4-3-5-8(6-7)9-2/h3-6H,1-2H3
InchiKey:	HCQVSQDSAZSABA-UHFFFAOYSA-N
Formula:	C8H10S
SMILES:	CSc1cccc(C)c1
Mol. weight [g/mol]:	138.23
CAS:	4886-77-5

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	8.50	eV	NIST Webbook
ie	8.00	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	1213.00		NIST Webbook
rinpol	1213.00		NIST Webbook
tb	482.88	K	Joback Method
tc	718.95	K	Joback Method
tf	253.26	K	Joback Method
vc	0.429	m ³ /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

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=C4886775&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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