

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

Other names:	Anisole, o-(methylthio)- o-Methoxyphenyl methyl sulfide 1-Methoxy-2-methylthiobenzene 2-Methoxythiophenol, S-methyl- 1-Methoxy-2-(methylsulfanyl)benzene
Inchi:	InChI=1S/C8H10OS/c1-9-7-5-3-4-6-8(7)10-2/h3-6H,1-2H3
InchiKey:	YCUXDIFPTHNTSR-UHFFFAOYSA-N
Formula:	C8H10OS
SMILES:	COc1ccccc1SC
Mol. weight [g/mol]:	154.23
CAS:	2388-73-0

Physical Properties

Property code	Value	Unit	Source
gf	47.38	kJ/mol	Joback Method
hf	-73.74	kJ/mol	Joback Method
hfus	15.45	kJ/mol	Joback Method
hvap	45.57	kJ/mol	Joback Method
ie	8.05	eV	NIST Webbook
log10ws	-2.34		Crippen Method
logp	2.417		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
rinpol	1350.80		NIST Webbook
tb	505.30	K	Joback Method
tc	738.56	K	Joback Method
tf	275.49	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.37	J/mol×K	505.30	Joback Method
cpg	257.93	J/mol×K	544.18	Joback Method

cpg	269.82	J/mol×K	583.05	Joback Method
cpg	281.04	J/mol×K	621.93	Joback Method
cpg	291.60	J/mol×K	660.81	Joback Method
cpg	301.49	J/mol×K	699.69	Joback Method
cpg	310.72	J/mol×K	738.56	Joback Method

Sources

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=C2388730&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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