

Benzenethiol, 2-methoxy-

Other names:	2-Methoxybenzenethiol 2-Methoxythiophenol o-Methoxythiophenol Benzenethiol, o-methoxy- o-Methoxybenzenethiol Thioguaiacol
Inchi:	InChI=1S/C7H8OS/c1-8-6-4-2-3-5-7(6)/h2-5,9H,1H3
InchiKey:	DSCJETUEDFKYGN-UHFFFAOYSA-N
Formula:	C7H8OS
SMILES:	COC1ccccc1S
Mol. weight [g/mol]:	140.20
CAS:	7217-59-6

Physical Properties

Property code	Value	Unit	Source
gf	35.23	kJ/mol	Joback Method
hf	-56.49	kJ/mol	Joback Method
hfus	12.77	kJ/mol	Joback Method
hvap	43.26	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.984		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
pc	4288.66	kPa	Joback Method
rinpol	1237.20		NIST Webbook
rinpol	1237.20		NIST Webbook
tb	476.50	K	Joback Method
tc	714.44	K	Joback Method
tf	266.28	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.69	J/mol×K	476.50	Joback Method

cpg	213.83	J/mol×K	516.16	Joback Method
cpg	224.36	J/mol×K	555.81	Joback Method
cpg	234.28	J/mol×K	595.47	Joback Method
cpg	243.60	J/mol×K	635.12	Joback Method
cpg	252.33	J/mol×K	674.78	Joback Method
cpg	260.48	J/mol×K	714.44	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.20	K	1.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7217596&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

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

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