Phenol, 2-(methylthio)-

Other names:	Phenol, o-(methylthio)-
	o-(Methylthio)phenol
	o-Hydroxythioanisole
	2-(Methylthio)phenol
	2-(Methylmercapto)phenol
	2-(Methylsulfanyl)phenol
Inchi:	InChI=1S/C7H8OS/c1-9-7-5-3-2-4-6(7)8/h2-5,8H,1H3
InchiKey:	SOOARYARZPXNAL-UHFFFAOYSA-N
Formula:	C7H8OS
SMILES:	CSc1ccccc1O
Mol. weight [g/mol]:	140.20
CAS:	1073-29-6

Physical Properties

Property code	Value	Unit	Source
gf	-1.03	kJ/mol	Joback Method
hf	-86.72	kJ/mol	Joback Method
hfus	17.84	kJ/mol	Joback Method
hvap	53.28	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	2.114		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
pc	5153.45	kPa	Joback Method
rinpol	1175.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1190.60		NIST Webbook
tb	535.64	K	Joback Method
tc	788.76	K	Joback Method
tf	341.19	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.91	J/mol×K	535.64	Joback Method
cpg	237.66	J/mol×K	577.83	Joback Method
cpg	247.52	J/mol×K	620.01	Joback Method
cpg	256.57	J/mol×K	662.20	Joback Method
cpg	264.90	J/mol×K	704.39	Joback Method
cpg	272.61	J/mol×K	746.57	Joback Method
cpg	279.79	J/mol×K	788.76	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.70	K	2.80	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1073296&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
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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