

4-Mercaptophenol

Other names:	p-Hydroxythiophenol 4-Hydroxythiophenol Phenol, 4-mercapto- p-Mercaptophenol Hydroquinone, monothio- Monothiohydroquinone Phenol, p-mercapto- Thiohydroquinone USAF B-57 4-Hydroxybenzenethiol NSC 46192 p-Hydroxybenzenethiol 4-Sulfanylphenol
Inchi:	InChI=1S/C6H6OS/c7-5-1-3-6(8)4-2-5/h1-4,7-8H
InchiKey:	BXAVKNRWVKUTLY-UHFFFAOYSA-N
Formula:	C6H6OS
SMILES:	Oc1ccc(S)cc1
Mol. weight [g/mol]:	126.18
CAS:	637-89-8

Physical Properties

Property code	Value	Unit	Source
gf	-13.18	kJ/mol	Joback Method
hf	-69.47	kJ/mol	Joback Method
hfus	15.16	kJ/mol	Joback Method
hvap	50.98	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.681		Crippen Method
mcvol	93.860	ml/mol	McGowan Method
pc	6400.00	kPa	Joback Method
rinpol	1319.40		NIST Webbook
rinpol	1319.40		NIST Webbook
tb	506.84	K	Joback Method
tc	766.12	K	Joback Method
tf	331.98	K	Joback Method
vc	0.283	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.39	J/mol×K	506.84	Joback Method
cpg	193.79	J/mol×K	550.05	Joback Method
cpg	202.28	J/mol×K	593.27	Joback Method
cpg	209.98	J/mol×K	636.48	Joback Method
cpg	216.99	J/mol×K	679.69	Joback Method
cpg	223.42	J/mol×K	722.90	Joback Method
cpg	229.38	J/mol×K	766.12	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	422.70	K	3.30	NIST Webbook
tbrp	440.20	K	6.00	NIST Webbook
tbrp	408.20	K	1.50	NIST Webbook

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=C637898&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
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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