Benzenethiol, 3-methyl-

Other names:	3-Mercaptotoluene
	3-Methylbenzenethiol
	3-Methylthiophenol
	3-Thiocresol
	NSC 81219
	USAF EK-2680
	m-Mercaptotoluene
	m-Methylbenzenethiol
	m-Methylthiophenol
	m-Thiocresol
	m-Toluenethiol
	m-Tolylmercaptan
	m-Tolylthiol
	toluene-3-thiol
Inchi:	InChI=1S/C7H8S/c1-6-3-2-4-7(8)5-6/h2-5,8H,1H3
InchiKey:	WRXOZRLZDJAYDR-UHFFFAOYSA-N
Formula:	C7H8S
SMILES:	Cc1cccc(S)c1
Mol. weight [g/mol]:	124.20
CAS:	108-40-7

Physical Properties

Property code	Value	Unit	Source
gf	140.23	kJ/mol	Joback Method
hf	75.73	kJ/mol	Joback Method
hfus	11.58	kJ/mol	Joback Method
hvap	40.85	kJ/mol	Joback Method
ie	8.44	eV	NIST Webbook
log10ws	-2.46		Crippen Method
logp	2.284		Crippen Method
mcvol	102.080	ml/mol	McGowan Method
pc	4385.77	kPa	Joback Method
tb	468.20	K	NIST Webbook
tc	694.66	K	Joback Method
tf	244.05	K	Joback Method
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.55	J/mol×K	454.08	Joback Method
cpg	192.97	J/mol×K	494.18	Joback Method
cpg	203.66	J/mol×K	534.27	Joback Method
cpg	213.64	J/mol×K	574.37	Joback Method
cpg	222.96	J/mol×K	614.47	Joback Method
cpg	231.63	J/mol×K	654.56	Joback Method
cpg	239.70	J/mol×K	694.66	Joback Method
hvapt	48.70	kJ/mol	425.50	NIST Webbook
hvapt	47.10	kJ/mol	425.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45987e+01
Coeff. B	-3.96098e+03
Coeff. C	-7.13230e+01
Temperature range (K), min.	348.10
Temperature range (K), max.	497.82

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=C108407&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume