1,2-Benzenedithiol, 4-methyl-

Other names:	Toluene-3,4-dithiol
	3,4-Dimercaptotoluene
	3,4-Dimercaptotoluol
	4-Methyl-1,2-benzenedithiol
	Dithiol
	1,2-Dimercapto-4-methylbenzene
	4-Methyl-1,2-dimercaptobenzene
	USAF B-59
	NSC 5391
Inchi:	InChI=1S/C7H8S2/c1-5-2-3-6(8)7(9)4-5/h2-4,8-9H,1H3
InchiKey:	NIAAGQAEVGMHPM-UHFFFAOYSA-N
Formula:	C7H8S2
SMILES:	Cc1ccc(S)c(S)c1
Mol. weight [g/mol]:	156.27
CAS:	496-74-2

Physical Properties

Property code	Value	Unit	Source
gf	159.99	kJ/mol	Joback Method
hf	102.74	kJ/mol	Joback Method
hfus	15.23	kJ/mol	Joback Method
hvap	48.25	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.572		Crippen Method
mcvol	118.430	ml/mol	McGowan Method
pc	4684.89	kPa	Joback Method
tb	521.92	K	Joback Method
tc	789.57	K	Joback Method
tf	293.03	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	222.24	J/mol×K	521.92	Joback Method
cpg	233.51	J/mol×K	566.53	Joback Method
cpg	243.99	J/mol×K	611.14	Joback Method
cpg	253.71	J/mol×K	655.74	Joback Method
cpg	262.70	J/mol×K	700.35	Joback Method
cpg	270.99	J/mol×K	744.96	Joback Method
cpg	278.62	J/mol×K	789.57	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	409.20	K	2.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C496742&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume