

Benzenethiol, 4-methyl-

Other names:	1-Mercapto-4-methylbenzene 4-Methylbenzenethiol 4-Methylphenyl mercaptan 4-Methylthiophenol 4-Thiocresol 4-Toluenethiol NSC 2227 USAF EK-510 p-Mercaptotoluene p-Methylbenzenethiol p-Methylbenzenthionol p-Methylphenyl mercaptan p-Methylthiophenol p-Thiocresol p-Thiolcresol p-Toluenethiol p-Tolyl mercaptan p-Tolylthiol p-Tolylthiophenol toluene-4-thiol
Inchi:	InChI=1S/C7H8S/c1-6-2-4-7(8)5-3-6/h2-5,8H,1H3
InchiKey:	WLHCBQAPPJAUW-UHFFFAOYSA-N
Formula:	C7H8S
SMILES:	Cc1ccc(S)cc1
Mol. weight [g/mol]:	124.20
CAS:	106-45-6

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	8.00	eV	NIST Webbook
ie	8.33	eV	NIST Webbook
log10ws	-2.46		Crippen Method
logp	2.284		Crippen Method

mvol	102.080	ml/mol	McGowan Method
pc	4385.77	kPa	Joback Method
rinpol	1048.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1047.00		NIST Webbook
tb	468.20	K	NIST Webbook
tc	694.66	K	Joback Method
tf	244.05	K	Joback Method
vc	0.373	m ³ /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	48.10	kJ/mol	425.00	NIST Webbook
hvapt	46.50	kJ/mol	425.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45817e+01
Coeff. B	-3.95478e+03
Coeff. C	-7.12680e+01
Temperature range (K), min.	317.15
Temperature range (K), max.	497.88

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=C106456&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/ci9903071

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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