O-TOLUENETHIOL

Other names:	2-Methylbenzenethiol
	2-Methylbenzothiol
	2-Methylphenylthiol
	2-Methylthiophenol
	2-Toluenethiol
	Benzenethiol, 2-methyl-
	NSC 80655
	USAF EK-2676
	o-Mercaptotoluene
	o-Methylbenzenethiol
	o-Methylthiophenol
	o-Thiocresol
	o-Tolyl mercaptan
	toluene-2-thiol
Inchi:	InChI=1S/C7H8S/c1-6-4-2-3-5-7(6)8/h2-5,8H,1H3
InchiKey:	LXUNZSDDXMPKLP-UHFFFAOYSA-N
Formula:	C7H8S
SMILES:	Cc1ccccc1S
Mol. weight [g/mol]:	124.21
CAS:	137-06-4

Physical Properties

Property code	Value	Unit	Source
af	0.3145		Cheméo Relay (1.0)
gf	140.23	kJ/mol	Joback Method
hf	77.93	kJ/mol	Cheméo Relay (1.0)
hfus	11.58	kJ/mol	Joback Method
hvap	53.67	kJ/mol	Cheméo Relay (1.0)
ie	8.31	eV	NIST Webbook
log10ws	-2.79		Cheméo Relay (1.0)
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	694.72	K	Cheméo Relay (1.0)
tf	260.76	K	Cheméo Relay (1.0)
vc	0.352	m3/kmol	Cheméo Relay (1.0)

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	424.50	NIST Webbook
hvapt	46.60	kJ/mol	420.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45809e+01
Coeff. B	-4.10903e+03
Coeff. C	-5.57550e+01
Temperature range (K), min.	343.23
Temperature range (K), max.	499.04

Sources

Cheméo Relay (1.0):

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1854.mol

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0, beta):

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C137064&Units=SI

Legend

af:	Acentric Factor
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