

4-Methoxy-«alpha»-toluenethiol

Other names:	p-Methoxy-«alpha»-toluenethiol Benzenemethanethiol, 4-methoxy- p-Methoxybenzyl mercaptan p-Methoxybenzylthiol
Inchi:	InChI=1S/C8H10OS/c1-9-8-4-2-7(6-10)3-5-8/h2-5,10H,6H2,1H3
InchiKey:	PTDVPWWJRCOIIO-UHFFFAOYSA-N
Formula:	C8H10OS
SMILES:	COc1ccc(CS)cc1
Mol. weight [g/mol]:	154.23
CAS:	6258-60-2

Physical Properties

Property code	Value	Unit	Source
gf	43.65	kJ/mol	Joback Method
hf	-77.13	kJ/mol	Joback Method
hfus	15.36	kJ/mol	Joback Method
hvap	45.49	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.125		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
pc	3796.32	kPa	Joback Method
rinpol	1359.90		NIST Webbook
tb	499.38	K	Joback Method
tc	733.05	K	Joback Method
tf	277.55	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.64	J/mol×K	499.38	Joback Method
cpg	256.12	J/mol×K	538.33	Joback Method
cpg	267.90	J/mol×K	577.27	Joback Method
cpg	278.99	J/mol×K	616.22	Joback Method

cpg	289.41	J/mol×K	655.16	Joback Method
cpg	299.18	J/mol×K	694.11	Joback Method
cpg	308.29	J/mol×K	733.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6258602&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
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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