Benzenesulfonic acid, 4-methyl-

Other names:	4-methylbenzenesulfonic acid
	4-toluenesulfonic acid
	Ar-Toluenesulfonic acid
	Benzenesulfonic acid, methyl-
	Cyclophil P T S A
	Cyzac 4040
	Eltesol
	K-Cure 1040
	Kyselina p-toluenesulfonova
	Kyselina p-toluensulfonova
	Manro PTSA 65 E
	Manro PTSA 65 H
	Manro PTSA 65 LS
	Methylbenzenesulfonic acid
	NSC 167068
	Nacure 1040
	PTSA
	Toluene-4-sulfonic acid
	Toluene-p-sulfonate
	Toluenesulfonic acid
	Tosic acid
	Tosylic acid
	Tsa-hp
	Tsa-mh
	p-Methylbenzenesulfonic acid
	p-Methylphenylsulfonic acid
	p-Toluenesulfonate
	p-Toluenesulphonic acid
	p-Toluolenesulfonic acid
	p-Tolylsulfonic acid
	p-toluenesulfonic acid
	toluene-4-sulphonic acid
Inchi:	InChI=1S/C7H8O3S/c1-6-2-4-7(5-3-6)11(8,9)10/h2-5H,1H3,(H,8,9,10)
InchiKey:	JOXIMZWYDAKGHI-UHFFFAOYSA-N
Formula:	C7H8O3S
SMILES:	Cc1ccc(S(=O)(=O)O)cc1
Mol. weight [g/mol]:	172.20
CAS:	104-15-4

Physical Properties

Property code	Value	Unit	Source
gf	-494.52	kJ/mol	Joback Method
hf	-568.33	kJ/mol	Joback Method
hfus	23.00	kJ/mol	Joback Method
hvap	69.43	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.242		Crippen Method
mcvol	119.690	ml/mol	McGowan Method
pc	5678.82	kPa	Joback Method
tb	531.18	K	Joback Method
tc	726.34	K	Joback Method
tf	306.97	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.31	J/mol×K	531.18	Joback Method
cpg	265.14	J/mol×K	563.71	Joback Method
cpg	274.44	J/mol×K	596.23	Joback Method
cpg	283.20	J/mol×K	628.76	Joback Method
cpg	291.44	J/mol×K	661.29	Joback Method
cpg	299.15	J/mol×K	693.81	Joback Method
cpg	306.34	J/mol×K	726.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Effect of Hydrogen Bond Donor on the Physical Properties of Benzyltriethylammonium Chloride Based Deep Eutectic Solvents and Thermodynamic Analysis of Biocative Conformation	https://www.doi.org/10.1021/acs.jced.6b00486
Solubility Increment and Thermodynamic Analysis of Bioactive Solubility of Methylbenzene Sulfonic Acid in 2-Ethylhexyl Acetate Synthesis Catalyst and Cosolvent Mixtures:	https://www.doi.org/10.1021/acs.jced.9b00717
Thermodynamic Models for Supercritical Carbon Dioxide and Modified Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je700639s
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume