Benzenesulfonamide, 4-methyl-

Other names:	4-Methylbenzenesulfonamide
	4-Toluenesulfanamide
	4-Toluenesulfonamide
	NSC 9908
	Tolouen-4-sulfonamide
	Toluene-4-sulfonamide
	Toluene-p-sulfonamide
	Toluene-p-sulphonamide
	Tolylsulfonamide
	Tosylamide
	Uniplex 173
	p-Methylbenzenesulfonamide
	p-Toluenesulfamide
	p-Toluenesulfanamide
	p-Toluenesulfonamide
	p-Toluenesulfonylamide
	p-Toluenesulphonamide
	p-Tolylsulfonamide
	p-Tosylamide
	para-Toluenesulfonamide
	toluene-4-sulphonamide
Inchi:	InChI=1S/C7H9NO2S/c1-6-2-4-7(5-3-6)11(8,9)10/h2-5H,1H3,(H2,8,9,10)
InchiKey:	LMYRWZFENFIFIT-UHFFFAOYSA-N
Formula:	C7H9NO2S
SMILES:	Cc1ccc(S(N)(=O)=O)cc1
Mol. weight [g/mol]:	171.22
CAS:	70-55-3

Physical Properties

Property code	Value	Unit	Source
gf	-291.25	kJ/mol	Joback Method
hf	-382.31	kJ/mol	Joback Method
hfus	23.93	kJ/mol	Enthalpies of combustion and formation of benzenesulfonamide and some of its derivatives
hvap	63.39	kJ/mol	Joback Method

log10ws	-1.74		Aqueous Solubility Prediction Method
log10ws	-1.74		Estimated Solubility Method
logp	0.642		Crippen Method
mcvol	123.800	ml/mol	McGowan Method
pc	5390.71	kPa	Joback Method
rinpol	1692.00		NIST Webbook
rinpol	1692.00		NIST Webbook
tb	511.53	K	Joback Method
tc	731.06	K	Joback Method
tf	339.25 ± 0.50	K	NIST Webbook
tf	411.65	K	Aqueous Solubility Prediction Method
tf	338.25 ± 0.70	K	NIST Webbook
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.34	J/mol×K	511.53	Joback Method
cpg	273.28	J/mol×K	548.12	Joback Method
cpg	284.51	J/mol×K	584.71	Joback Method
cpg	295.04	J/mol×K	621.30	Joback Method
cpg	304.87	J/mol×K	657.89	Joback Method
cpg	314.01	J/mol×K	694.48	Joback Method
cpg	322.46	J/mol×K	731.06	Joback Method

Sources

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

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

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Enthalpies of combustion and formation of benzenesulfonamide and some of its derivatives: https://www.doi.org/10.1016/j.jct.2011.11.026

Solubility of p-Toluenesulfonamide in Pure and Modified Supercritical Carbon Dioxide: https://www.doi.org/10.1021/je8008842

Solubility and Mixing Thermodynamics Properties of p-Toluenesulfonamide and o-Toluenesulfonamide in Seven Monosolvents at Different Temperatures: https://www.doi.org/10.1021/acs.jced.7b00714

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C70553&Units=SI

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