Benzenesulfonamide, 2-methyl-

Other names:	2-Methylbenzenesulfonamide
	2-Tolylsulfonamide
	2-toluenesulfonamide
	NSC 2185
	OTS amide
	Ortho-toluol-sulfonamid
	Toluene-2-sulfonamide
	o-Methylbenzenesulfonamide
	o-Toluenesulfonamide
	ortho-Toluenesulfonamide
	toluene-2-sulphonamide
Inchi:	InChI=1S/C7H9NO2S/c1-6-4-2-3-5-7(6)11(8,9)10/h2-5H,1H3,(H2,8,9,10)
InchiKey:	YCMLQMDWSXFTIF-UHFFFAOYSA-N
Formula:	C7H9NO2S
SMILES:	Cc1ccccc1S(N)(=O)=O
Mol. weight [g/mol]:	171.22
CAS:	88-19-7

Physical Properties

Property code	Value	Unit	Source
gf	-291.25	kJ/mol	Joback Method
hf	-382.31	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Enthalpies of combustion and formation of benzenesulfonamide and some of its derivatives
hvap	63.39	kJ/mol	Joback Method
log10ws	-2.02		Aqueous Solubility Prediction Method
logp	0.642		Crippen Method
mcvol	123.800	ml/mol	McGowan Method
pc	5390.71	kPa	Joback Method
tb	511.53	K	Joback Method
tc	731.06	K	Joback Method
tf	429.30	K	Aqueous Solubility Prediction Method

tt	427.35	K	Solubility Measurement and Thermodynamic Modeling for o-Toluenesulfonamide in 16 Solvents from T = 273.15 to 323.85 K
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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C88197&Units=SI

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

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

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

Solubility Measurement and Thermodynamic Modeling for o-Toluenesulfonamide in 16 Solvents from T = 273.15 to 323.85 K: https://www.doi.org/10.1021/acs.jced.9b00445

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

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

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
tt:	Triple Point Temperature
vc:	Critical Volume