Benzenemethanesulfonamide

Other names:	«alpha»-Toluenesulfonamide
	Benzylsulfonamide
	Methanesulfonamide, 1-phenyl-
	Phenylmethanesulfonamide
	Toluene-«omega»-sulfonamide
	Toluenesulfonamide, alpha-
	toluene-«alpha»-sulphonamide
Inchi:	InChI=1S/C7H9NO2S/c8-11(9,10)6-7-4-2-1-3-5-7/h1-5H,6H2,(H2,8,9,10)
InchiKey:	ABOYDMHGKWRPFD-UHFFFAOYSA-N
Formula:	C7H9NO2S
SMILES:	NS(=O)(=O)Cc1ccccc1
Mol. weight [g/mol]:	171.22
CAS:	4563-33-1

Physical Properties

Property code	Value	Unit	Source
gf	-281.62	kJ/mol	Joback Method
hf	-370.84	kJ/mol	Joback Method
hfus	24.50	kJ/mol	Joback Method
hvap	62.73	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	0.475		Crippen Method
mcvol	123.800	ml/mol	McGowan Method
pc	5511.44	kPa	Joback Method
tb	506.55	K	Joback Method
tc	724.87	K	Joback Method
tf	316.89	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.52	J/mol×K	506.55	Joback Method
cpg	273.85	J/mol×K	542.94	Joback Method

cpg	285.41	J/mol×K	579.32	Joback Method
cpg	296.20	J/mol×K	615.71	Joback Method
cpg	306.25	J/mol×K	652.10	Joback Method
cpg	315.56	J/mol×K	688.48	Joback Method
cpg	324.15	J/mol×K	724.87	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4563331&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume