4-Aminophenyl methyl sufhone

Other names: Benzenamine, 4-(methylsulfonyl)-
Aniline, p-(methylsulfonyl)-
4-(Methylsulfonyl)aniline
4-mesylaniline
Inchi: InChI=1S/C7H9NO2S/c1-11(9,10)7-4-2-6(8)3-5-7/h2-5H,8H2,1H3
InchiKey: XJEVFFNOMKXBLU-UHFFFAOYSA-N
Formula: C7H9NO2S
SMILES: CS(=O)(=O)c1ccc(N)cc1
Mol. weight [g/mol]: 171.22
CAS: 5470-49-5

Physical Properties

Property code	Value	Unit	Source
gf	-291.25	kJ/mol	Joback Method
hf	-382.31	kJ/mol	Joback Method
hfus	24.11	kJ/mol	Joback Method
hvap	63.39	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	0.672		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	329.41	K	Joback Method
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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5470495&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