Acetanilide, 4'-(methylsulfonyl)-

Inchi: InChI=1S/C9H11NO3S/c1-7(11)10-8-3-5-9(6-4-8)14(2,12)13/h3-6H,1-2H3,(H,10,11)
InchiKey: SJYUABJSWXGSAO-UHFFFAOYSA-N
Formula: C9H11NO3S
SMILES: CC(=O)Nc1ccc(S(C)(=O)=O)cc1
Mol. weight [g/mol]: 213.25
CAS: 22821-80-3

Physical Properties

Property code	Value	Unit	Source
gf	-380.39	kJ/mol	Joback Method
hf	-516.49	kJ/mol	Joback Method
hfus	30.79	kJ/mol	Joback Method
hvap	70.38	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.048		Crippen Method
mcvol	153.550	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
tb	588.80	K	Joback Method
tc	800.39	K	Joback Method
tf	371.28	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.25	J/mol×K	588.80	Joback Method
cpg	370.03	J/mol×K	624.07	Joback Method
cpg	382.00	J/mol×K	659.33	Joback Method
cpg	393.15	J/mol×K	694.60	Joback Method
cpg	403.50	J/mol×K	729.86	Joback Method
cpg	413.06	J/mol×K	765.13	Joback Method
cpg	421.84	J/mol×K	800.39	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22821803&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume