N-Acetylbenzenesulfonamide

Inchi: InChI=1S/C8H9NO3S/c1-7(10)9-13(11,12)8-5-3-2-4-6-8/h2-6H,1H3,(H,9,10)
InchiKey: JHKCSRBLMSDCML-UHFFFAOYSA-N
Formula: C8H9NO3S
SMILES: CC(=O)NS(=O)(=O)c1ccccc1
Mol. weight [g/mol]: 199.23
CAS: 5661-14-3

Physical Properties

Property code	Value	Unit	Source
chs	-4304.10	kJ/mol	NIST Webbook
gf	-379.18	kJ/mol	Joback Method
hf	-484.38	kJ/mol	Joback Method
hfs	-732.20	kJ/mol	NIST Webbook
hfus	28.59	kJ/mol	Joback Method
hvap	67.49	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	0.511		Crippen Method
mcvol	139.460	ml/mol	McGowan Method
pc	4931.51	kPa	Joback Method
tb	560.94	K	Joback Method
tc	775.08	K	Joback Method
tf	347.49	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.58	J/mol×K	560.94	Joback Method
cpg	323.84	J/mol×K	596.63	Joback Method
cpg	335.29	J/mol×K	632.32	Joback Method
cpg	345.93	J/mol×K	668.01	Joback Method
cpg	355.78	J/mol×K	703.70	Joback Method
cpg	364.85	J/mol×K	739.39	Joback Method
cpg	373.15	J/mol×K	775.08	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=C5661143&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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