Benzenesulfonamide, 4-acetyl-

Other names: 4-Acetylbenzenesulfonamide
4-acetylbenzenesulphonamide
Inchi: InChI=1S/C8H9NO3S/c1-6(10)7-2-4-8(5-3-7)13(9,11)12/h2-5H,1H3,(H2,9,11,12)
InchiKey: CSATVXJBGFVJES-UHFFFAOYSA-N
Formula: C8H9NO3S
SMILES: CC(=O)c1ccc(S(N)(=O)=O)cc1
Mol. weight [g/mol]: 199.23
CAS: 1565-17-9

Physical Properties

Property code	Value	Unit	Source
gf	-411.75	kJ/mol	Joback Method
hf	-515.53	kJ/mol	Joback Method
hfus	28.30	kJ/mol	Joback Method
hvap	72.36	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	0.537		Crippen Method
mcvol	139.460	ml/mol	McGowan Method
pc	5138.68	kPa	Joback Method
rinpol	1984.00		NIST Webbook
rinpol	1984.00		NIST Webbook
tb	588.28	K	Joback Method
tc	812.24	K	Joback Method
tf	390.61	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.66	J/mol×K	588.28	Joback Method
cpg	331.33	J/mol×K	625.61	Joback Method
cpg	342.18	J/mol×K	662.93	Joback Method
cpg	352.23	J/mol×K	700.26	Joback Method
cpg	361.49	J/mol×K	737.59	Joback Method

cpg	369.96	J/mol×K	774.91	Joback Method
cpg	377.64	J/mol×K	812.24	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=C1565179&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume