N-acetylsulfanilamide

Inchi: InChI=1S/C8H10N2O3S/c1-6(11)10-7-2-4-8(5-3-7)14(9,12)13/h2-5H,1H3,(H,10,11)(H2,9
InchiKey: PKOFBDHYTMYVGJ-UHFFFAOYSA-N
Formula: C8H10N2O3S
SMILES: CC(=O)Nc1ccc(S(N)(=O)=O)cc1
Mol. weight [g/mol]: 214.25

Physical Properties

Property code	Value	Unit	Source
gf	-322.36	kJ/mol	Joback Method
hf	-462.06	kJ/mol	Joback Method
hfus	33.40	kJ/mol	Joback Method
hvap	78.80	kJ/mol	Joback Method
log10ws	-1.61		Aqueous Solubility Prediction Method
logp	0.292		Crippen Method
mcvol	149.440	ml/mol	McGowan Method
pc	5235.81	kPa	Joback Method
tb	638.45	K	Joback Method
tc	861.20	K	Joback Method
tf	492.65	K	Aqueous Solubility Prediction Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.52	J/mol×K	638.45	Joback Method
cpg	377.00	J/mol×K	675.58	Joback Method
cpg	387.62	J/mol×K	712.70	Joback Method
cpg	397.38	J/mol×K	749.83	Joback Method
cpg	406.29	J/mol×K	786.95	Joback Method
cpg	414.37	J/mol×K	824.08	Joback Method
cpg	421.62	J/mol×K	861.20	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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