4-sulfamoylbenzamide

Inchi: InChI=1S/C7H8N2O3S/c8-7(10)5-1-3-6(4-2-5)13(9,11)12/h1-4H,(H2,8,10)(H2,9,11,12)
InchiKey: MWFFIRCXGDGFQB-UHFFFAOYSA-N
Formula: C7H8N2O3S
SMILES: NC(=O)c1ccc(S(N)(=O)=O)cc1
Mol. weight [g/mol]: 200.22

Physical Properties

Property code	Value	Unit	Source
gf	-353.72	kJ/mol	Joback Method
hf	-461.10	kJ/mol	Joback Method
hfus	30.91	kJ/mol	Joback Method
hvap	80.78	kJ/mol	Joback Method
log10ws	-2.30		Aqueous Solubility Prediction Method
logp	-0.567		Crippen Method
mcvol	135.350	ml/mol	McGowan Method
pc	6482.71	kPa	Joback Method
tb	637.93	K	Joback Method
tc	873.43	K	Joback Method
tf	462.60	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.52	J/mol×K	637.93	Joback Method
cpg	335.85	J/mol×K	677.18	Joback Method
cpg	345.33	J/mol×K	716.43	Joback Method
cpg	353.96	J/mol×K	755.68	Joback Method
cpg	361.74	J/mol×K	794.93	Joback Method
cpg	368.70	J/mol×K	834.18	Joback Method
cpg	374.83	J/mol×K	873.43	Joback Method

Sources

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

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