benzene-1,3-disulfonamide

Inchi: InChI=1S/C6H8N2O4S2/c7-13(9,10)5-2-1-3-6(4-5)14(8,11)12/h1-4H,(H2,7,9,10)(H2,8,11
InchiKey: HUYYFHGIHVULSU-UHFFFAOYSA-N
Formula: C6H8N2O4S2
SMILES: NS(=O)(=O)c1cccc(S(N)(=O)=O)c1
Mol. weight [g/mol]: 236.27

Physical Properties

Property code	Value	Unit	Source
gf	-701.76	kJ/mol	Joback Method
hf	-781.23	kJ/mol	Joback Method
hfus	38.10	kJ/mol	Joback Method
hvap	90.44	kJ/mol	Joback Method
log10ws	-2.17		Aqueous Solubility Prediction Method
logp	-1.019		Crippen Method
mcvol	147.780	ml/mol	McGowan Method
pc	9001.58	kPa	Joback Method
tb	608.96	K	Joback Method
tc	832.10	K	Joback Method
tf	439.96	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.43	J/mol×K	608.96	Joback Method
cpg	357.43	J/mol×K	646.15	Joback Method
cpg	367.58	J/mol×K	683.34	Joback Method
cpg	376.86	J/mol×K	720.53	Joback Method
cpg	385.28	J/mol×K	757.72	Joback Method
cpg	392.80	J/mol×K	794.91	Joback Method
cpg	399.42	J/mol×K	832.10	Joback Method

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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