4-nitrobenzenesulfonamide

Other names: benzenesulfonamide, 4-nitro-
Inchi: InChI=1S/C6H6N2O4S/c7-13(11,12)6-3-1-5(2-4-6)8(9)10/h1-4H,(H2,7,11,12)
InchiKey: QWKKYJLAUWFPDB-UHFFFAOYSA-N
Formula: C6H6N2O4S
SMILES: NS(=O)(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 202.19

Physical Properties

Property code	Value	Unit	Source
gf	-264.12	kJ/mol	Joback Method
hf	-372.43	kJ/mol	Joback Method
hfus	29.77	kJ/mol	Determination of the energies of combustion and enthalpies of formation of nitrobenzenesulfonamides by rotating-bomb combustion calorimetry
hvap	77.76	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	0.242		Crippen Method
mcvol	127.130	ml/mol	McGowan Method
pc	6359.24	kPa	Joback Method
tb	640.49	K	Joback Method
tc	890.70	K	Joback Method
tf	453.61	K	Determination of the energies of combustion and enthalpies of formation of nitrobenzenesulfonamides by rotating-bomb combustion calorimetry
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.72	J/mol×K	849.00	Joback Method

cpg	301.69	J/mol×K	640.49	Joback Method
cpg	311.72	J/mol×K	682.19	Joback Method
cpg	320.82	J/mol×K	723.89	Joback Method
cpg	329.01	J/mol×K	765.59	Joback Method
cpg	336.31	J/mol×K	807.30	Joback Method
cpg	348.26	J/mol×K	890.70	Joback Method
cpl	219.98	J/mol×K	298.15	Determination of the energies of combustion and enthalpies of formation of nitrobenzenesulfonamides by rotating-bomb combustion calorimetry

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination of the energies of combustion and enthalpies of formation of nitrobenzenesulfonamides by rotating-bomb combustion calorimetry:	https://www.doi.org/10.1016/j.jct.2009.10.003
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
cpl:	Liquid phase 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