M-nitrobenzenesulfonamide

Other names:	3-Nitrobenzolesulfamide 3-nitrobenzenesulfonamide Benzenesulfonamide, m-nitro- benzenesulfonamide, 3-nitro- m-nitrobenzenesulphonamide
Inchi:	InChI=1S/C6H6N2O4S/c7-13(11,12)6-3-1-2-5(4-6)8(9)10/h1-4H,(H2,7,11,12)
InchiKey:	TXTQURPQLVHJRE-UHFFFAOYSA-N
Formula:	C6H6N2O4S
SMILES:	NS(=O)(=O)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	202.19

Physical Properties

Property code	Value	Unit	Source
hf	-211.57	kJ/mol	Cheméo Relay (1.0)
hfus	31.47	kJ/mol	Determination of the energies of combustion and enthalpies of formation of nitrobenzenesulfonamides by rotating-bomb combustion calorimetry
hvap	89.00	kJ/mol	Cheméo Relay (1.0)
ie	10.12	eV	Cheméo Relay (1.0)
log10ws	-2.46		Cheméo Relay (1.0)
logp	0.242		Crippen Method
mcvol	127.130	ml/mol	McGowan Method
tb	578.61	K	Cheméo Relay (1.0)
tf	435.65 ± 1.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	342.72	J/mol×K	849.00	Joback Method
cpg	348.26	J/mol×K	890.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121528&Units=SI
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
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

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point