2-methyl-5-nitrobenzenesulfonic acid

Other names: p-nitrotoluene-o-sulfonic acid
Inchi: InChI=1S/C7H7NO5S/c1-5-2-3-6(8(9)10)4-7(5)14(11,12)13/h2-4H,1H3,(H,11,12,13)
InchiKey: ZDTXQHVBLWYPHS-UHFFFAOYSA-N
Formula: C7H7NO5S
SMILES: Cc1ccc([N+](=O)[O-])cc1S(=O)(=O)O
Mol. weight [g/mol]: 217.20

Physical Properties

Property code	Value	Unit	Source
hf	-435.41	kJ/mol	Cheméo Relay (1.0)
hfus	33.98	kJ/mol	Joback Method
hvap	104.11	kJ/mol	Cheméo Relay (1.0)
ie	10.22	eV	Cheméo Relay (1.0)
log10ws	-1.33		Cheméo Relay (1.0)
logp	1.150		Crippen Method
mcvol	137.110	ml/mol	McGowan Method
tb	581.40	K	Cheméo Relay (1.0)
tf	457.69	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.98	J/mol×K	688.00	Joback Method
cpg	346.74	J/mol×K	724.62	Joback Method
cpg	354.78	J/mol×K	761.24	Joback Method
cpg	362.11	J/mol×K	797.85	Joback Method
cpg	368.74	J/mol×K	834.47	Joback Method
cpg	374.66	J/mol×K	871.09	Joback Method
cpg	379.89	J/mol×K	907.71	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Investigation the solubility difference of sodium 4-nitrotoluene-2-sulfonate and 4-nitrotoluene-2-sulfonic acid in (sulfuric acid + water) system:	https://www.doi.org/10.1016/j.fluid.2013.08.023
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

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