5-Nitro-o-toluene sulfonic acid

Inchi: InChI=1S/C7H7NO5S/c1-5-4-6(8(9)10)2-3-7(5)14(11,12)13/h2-4H,1H3,(H,11,12,13)
InchiKey: XCSZUHHAYFILGO-UHFFFAOYSA-N
Formula: C7H7NO5S
SMILES: Cc1cc([N+](=O)[O-])ccc1S(=O)(=O)O
Mol. weight [g/mol]: 217.20

Physical Properties

Property code	Value	Unit	Source
gf	-468.60	kJ/mol	Joback Method
hf	-590.56	kJ/mol	Joback Method
hfus	33.98	kJ/mol	Joback Method
hvap	86.68	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.150		Crippen Method
mcvol	137.110	ml/mol	McGowan Method
pc	5653.23	kPa	Joback Method
tb	688.00	K	Joback Method
tc	907.71	K	Joback Method
tf	463.10	K	Joback Method
vc	0.546	m3/kmol	Joback Method

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000354&Units=SI

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