3-Amino-p-toluene sulfonic acid

Inchi: InChI=1S/C7H9NO3S/c1-5-2-3-7(6(8)4-5)12(9,10)11/h2-4H,8H2,1H3,(H,9,10,11)
InchiKey: FJHGMUDVUAXUEK-UHFFFAOYSA-N
Formula: C7H9NO3S
SMILES: Cc1ccc(S(=O)(=O)O)c(N)c1
Mol. weight [g/mol]: 187.22

Physical Properties

Property code	Value	Unit	Source
gf	-437.70	kJ/mol	Joback Method
hf	-546.01	kJ/mol	Joback Method
hfus	27.81	kJ/mol	Joback Method
hvap	80.73	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	0.824		Crippen Method
mcvol	129.670	ml/mol	McGowan Method
pc	6056.11	kPa	Joback Method
tb	608.69	K	Joback Method
tc	813.58	K	Joback Method
tf	402.75	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.73	J/mol×K	608.69	Joback Method
cpg	315.24	J/mol×K	642.84	Joback Method
cpg	324.16	J/mol×K	676.99	Joback Method
cpg	332.50	J/mol×K	711.14	Joback Method
cpg	340.25	J/mol×K	745.28	Joback Method
cpg	347.41	J/mol×K	779.43	Joback Method
cpg	354.00	J/mol×K	813.58	Joback Method

Sources

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=B6001362&Units=SI
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