2,3,5-Trinitrotoluene

Inchi: InChI=1S/C7H5N3O6/c1-4-2-5(8(11)12)3-6(9(13)14)7(4)10(15)16/h2-3H,1H3
InchiKey: DGSCKRLVSINLST-UHFFFAOYSA-N
Formula: C7H5N3O6
SMILES: Cc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1[N+](=O)[O-]
Mol. weight [g/mol]: 227.13
CAS: 609-74-5

Physical Properties

Property code	Value	Unit	Source
chs	-3447.00	kJ/mol	NIST Webbook
gf	198.23	kJ/mol	Joback Method
hf	-17.97	kJ/mol	Joback Method
hfus	40.84	kJ/mol	Joback Method
hvap	85.21	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	1.720		Crippen Method
mcvol	137.990	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
tb	856.70	K	Joback Method
tc	1146.44	K	Joback Method
tf	663.46	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.64	J/mol×K	856.70	Joback Method
cpg	379.23	J/mol×K	904.99	Joback Method
cpg	385.89	J/mol×K	953.28	Joback Method
cpg	391.69	J/mol×K	1001.57	Joback Method
cpg	396.66	J/mol×K	1049.86	Joback Method
cpg	400.88	J/mol×K	1098.15	Joback Method
cpg	404.39	J/mol×K	1146.44	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=C609745&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
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