2,4,6-TRINITROBENZOIC ACID

Other names:	2,4,6-Trinitrobenzoic acid
	Benzoic acid, trinitro-
	Benzoic acid, trinitro- (dry)
	Benzoic acid, trinitro- (wet)
	NSC 133453
	Trinitrobenzoic acid
	s-Trinitrobenzoic acid
	sym-Trinitrobenzoic acid
Inchi:	InChI=1S/C7H3N3O8/c11-7(12)6-4(9(15)16)1-3(8(13)14)2-5(6)10(17)18/h1-2H,(H,11,12)
InchiKey:	KAQBNBSMMVTKRN-UHFFFAOYSA-N
Formula:	C7H3N3O8
SMILES:	O=C(O)c1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	257.11

Physical Properties

Property code	Value	Unit	Source
chs	-2773.70	kJ/mol	NIST Webbook
hf	-242.93	kJ/mol	Cheméo Relay (1.0)
hfs	-409.70	kJ/mol	NIST Webbook
hfus	46.53	kJ/mol	Joback Method
hvap	107.53	kJ/mol	Cheméo Relay (1.0)
ie	10.95	eV	Cheméo Relay (1.0)
log10ws	-3.11		Cheméo Relay (1.0)
logp	1.109		Crippen Method
mcvol	145.430	ml/mol	McGowan Method
tb	553.61	K	Cheméo Relay (1.0)
tf	442.41	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.46	J/mol×K	1002.75	Joback Method
cpg	403.37	J/mol×K	1047.35	Joback Method
cpg	406.59	J/mol×K	1091.95	Joback Method

cpg	409.17	J/mol×K	1136.55	Joback Method
cpg	411.15	J/mol×K	1181.15	Joback Method
cpg	412.57	J/mol×K	1225.75	Joback Method
cpg	413.48	J/mol×K	1270.35	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C129668&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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