BENZOIC ACID, 2-CHLORO-3,5-DINITRO-

Other names: Benzoic acid, 2-chloro-3,5-dinitro-
Inchi: InChI=1S/C7H3ClN2O6/c8-6-4(7(11)12)1-3(9(13)14)2-5(6)10(15)16/h1-2H,(H,11,12)
InchiKey: ADTKEYLCJYYHHH-UHFFFAOYSA-N
Formula: C7H3ClN2O6
SMILES: O=C(O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1Cl
Mol. weight [g/mol]: 246.56

Physical Properties

Property code	Value	Unit	Source
hf	-280.50	kJ/mol	Cheméo Relay (1.0)
hfus	39.37	kJ/mol	Joback Method
hvap	104.83	kJ/mol	Cheméo Relay (1.0)
ie	10.41	eV	Cheméo Relay (1.0)
log10ws	-2.97		Cheméo Relay (1.0)
logp	1.855		Crippen Method
mcvol	140.250	ml/mol	McGowan Method
tb	513.70	K	NIST Webbook
tf	420.57	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.36	J/mol×K	888.34	Joback Method
cpg	354.38	J/mol×K	930.77	Joback Method
cpg	358.77	J/mol×K	973.20	Joback Method
cpg	362.57	J/mol×K	1015.64	Joback Method
cpg	365.81	J/mol×K	1058.07	Joback Method
cpg	368.52	J/mol×K	1100.50	Joback Method
cpg	370.74	J/mol×K	1142.93	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2497918&Units=SI
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