2-Chloro-3,5-dinitrobenzoic acid

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
CAS: 2497-91-8

Physical Properties

Property code	Value	Unit	Source
gf	-114.99	kJ/mol	Joback Method
hf	-287.76	kJ/mol	Joback Method
hfus	39.37	kJ/mol	Joback Method
hvap	96.43	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	1.855		Crippen Method
mcvol	140.250	ml/mol	McGowan Method
pc	4678.49	kPa	Joback Method
tb	513.70	K	NIST Webbook
tc	1142.93	K	Joback Method
tf	660.52	K	Joback Method
vc	0.557	m3/kmol	Joback Method

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

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=C2497918&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