Benzoic acid, 2-hydroxy-3,5-dinitro-

Other names:	Salicylic acid, 3,5-dinitro-
	2-Hydroxy-3,5-dinitrobenzoic acid
	3,5-Dinitro-2-hydroxybenzoic acid
	3,5-Dinitrosalicylic acid
Inchi:	InChI=1S/C7H4N2O7/c10-6-4(7(11)12)1-3(8(13)14)2-5(6)9(15)16/h1-2,10H,(H,11,12)
InchiKey:	LWFUFLREGJMOIZ-UHFFFAOYSA-N
Formula:	C7H4N2O7
SMILES:	O=C(O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1O
Mol. weight [g/mol]:	228.12
CAS:	609-99-4

Physical Properties

Property code	Value	Unit	Source
gf	-248.05	kJ/mol	Joback Method
hf	-437.86	kJ/mol	Joback Method
hfus	41.34	kJ/mol	Joback Method
hvap	104.40	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	0.907		Crippen Method
mcvol	133.880	ml/mol	McGowan Method
pc	6288.83	kPa	Joback Method
tb	926.55	K	Joback Method
tc	1184.19	K	Joback Method
tf	729.80	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.27	J/mol×K	926.55	Joback Method
cpg	374.26	J/mol×K	969.49	Joback Method
cpg	380.12	J/mol×K	1012.43	Joback Method
cpg	385.95	J/mol×K	1055.37	Joback Method
cpg	391.87	J/mol×K	1098.31	Joback Method

cpg	397.97	J/mol×K	1141.25	Joback Method
cpg	404.35	J/mol×K	1184.19	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=C609994&Units=SI

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