Benzoic acid, 3,4-dinitro-

Other names: 3,4-Dinitrobenzoic acid
Inchi: InChI=1S/C7H4N2O6/c10-7(11)4-1-2-5(8(12)13)6(3-4)9(14)15/h1-3H,(H,10,11)
InchiKey: OMVRRHJJQILIJX-UHFFFAOYSA-N
Formula: C7H4N2O6
SMILES: O=C(O)c1ccc([N+](=O)[O-])c([N+](=O)[O-])c1
Mol. weight [g/mol]: 212.12
CAS: 528-45-0

Physical Properties

Property code	Value	Unit	Source
gf	-93.43	kJ/mol	Joback Method
hf	-260.55	kJ/mol	Joback Method
hfus	35.56	kJ/mol	Joback Method
hsub	129.00 ± 2.00	kJ/mol	NIST Webbook
hvap	91.38	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	1.201		Crippen Method
mcvol	128.010	ml/mol	McGowan Method
pc	5029.93	kPa	Joback Method
tb	845.93	K	Joback Method
tc	1098.09	K	Joback Method
tf	618.08	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.23	J/mol×K	972.01	Joback Method
cpg	357.31	J/mol×K	1014.04	Joback Method
cpg	360.85	J/mol×K	1056.06	Joback Method
cpg	337.32	J/mol×K	845.93	Joback Method
cpg	343.27	J/mol×K	887.96	Joback Method
cpg	348.56	J/mol×K	929.98	Joback Method
cpg	363.88	J/mol×K	1098.09	Joback Method

hfust	24.60	kJ/mol	438.20	NIST Webbook
hsubt	126.00 ± 2.00	kJ/mol	382.50	NIST Webbook
hvapt	91.00 ± 3.00	kJ/mol	529.00	NIST Webbook
hvapt	91.00 ± 1.00	kJ/mol	521.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C528450&Units=SI
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

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
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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