Benzoic acid, 2,5-dinitro-

Other names: 2,5-Dinitrobenzoic acid
Inchi: InChI=1S/C7H4N2O6/c10-7(11)5-3-4(8(12)13)1-2-6(5)9(14)15/h1-3H,(H,10,11)
InchiKey: YKMDNKRCCODWMG-UHFFFAOYSA-N
Formula: C7H4N2O6
SMILES: O=C(O)c1cc([N+](=O)[O-])ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 212.12
CAS: 610-28-6

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
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	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	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	363.88	J/mol×K	1098.09	Joback Method

Sources

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=C610286&Units=SI
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
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