Benzonitrile, 3,5-dinitro-

Other names: 3,5-Dinitrobenzonitrile
Inchi: InChI=1S/C7H3N3O4/c8-4-5-1-6(9(11)12)3-7(2-5)10(13)14/h1-3H
InchiKey: SSDNULNTQAUNFQ-UHFFFAOYSA-N
Formula: C7H3N3O4
SMILES: N#Cc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 193.12
CAS: 4110-35-4

Physical Properties

Property code	Value	Unit	Source
ea	2.16 ± 0.10	eV	NIST Webbook
gf	305.49	kJ/mol	Joback Method
hf	169.14	kJ/mol	Joback Method
hfus	31.38	kJ/mol	Joback Method
hvap	78.44	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	1.375		Crippen Method
mcvol	121.950	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
tb	801.96	K	Joback Method
tc	1084.43	K	Joback Method
tf	572.32	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.41	J/mol×K	801.96	Joback Method
cpg	308.14	J/mol×K	849.04	Joback Method
cpg	314.11	J/mol×K	896.12	Joback Method
cpg	319.35	J/mol×K	943.19	Joback Method
cpg	323.93	J/mol×K	990.27	Joback Method
cpg	327.90	J/mol×K	1037.35	Joback Method
cpg	331.29	J/mol×K	1084.43	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=C4110354&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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