Benzenamine, 3,5-dinitro-

Other names: Aniline, 3,5-dinitro-
3,5-Dinitroaniline
Benzeneamine, 3,5-dinitro-
Inchi: InChI=1S/C6H5N3O4/c7-4-1-5(8(10)11)3-6(2-4)9(12)13/h1-3H,7H2
InchiKey: MPBZUKLDHPOCLS-UHFFFAOYSA-N
Formula: C6H5N3O4
SMILES: Nc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 183.12
CAS: 618-87-1

Physical Properties

Property code	Value	Unit	Source
chs	-3037.00	kJ/mol	NIST Webbook
gf	230.34	kJ/mol	Joback Method
hf	58.69	kJ/mol	Joback Method
hfs	-39.00	kJ/mol	NIST Webbook
hfus	32.48	kJ/mol	Joback Method
hvap	76.37	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	1.085		Crippen Method
mcvol	116.460	ml/mol	McGowan Method
pc	5015.69	kPa	Joback Method
rinpol	321.42		NIST Webbook
tb	749.53	K	Joback Method
tc	1034.10	K	Joback Method
tf	579.32	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.44	J/mol×K	749.53	Joback Method
cpg	306.66	J/mol×K	796.96	Joback Method
cpg	314.01	J/mol×K	844.39	Joback Method

cpg	320.54	J/mol×K	891.81	Joback Method
cpg	326.32	J/mol×K	939.24	Joback Method
cpg	331.39	J/mol×K	986.67	Joback Method
cpg	335.82	J/mol×K	1034.10	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=C618871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume