1,3-Diamino-2,4,6-trinitrobenzene

Inchi: InChI=1S/C6H5N5O6/c7-4-2(9(12)13)1-3(10(14)15)5(8)6(4)11(16)17/h1H,7-8H2
InchiKey: FZAZPMLWYUKRAE-UHFFFAOYSA-N
Formula: C6H5N5O6
SMILES: Nc1c([N+](=O)[O-])cc([N+](=O)[O-])c(N)c1[N+](=O)[O-]
Mol. weight [g/mol]: 243.13
CAS: 28930-29-2

Physical Properties

Property code	Value	Unit	Source
gf	313.08	kJ/mol	Joback Method
hf	58.78	kJ/mol	Joback Method
hfus	48.26	kJ/mol	Joback Method
hsub	143.50	kJ/mol	NIST Webbook
hvap	104.93	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	0.576		Crippen Method
mcvol	143.860	ml/mol	McGowan Method
pc	5304.68	kPa	Joback Method
tb	983.86	K	Joback Method
tc	1282.68	K	Joback Method
tf	831.23	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.06	J/mol×K	983.86	Joback Method
cpg	412.18	J/mol×K	1033.66	Joback Method
cpg	416.42	J/mol×K	1083.47	Joback Method
cpg	419.82	J/mol×K	1133.27	Joback Method
cpg	422.43	J/mol×K	1183.08	Joback Method
cpg	424.32	J/mol×K	1232.88	Joback Method
cpg	425.51	J/mol×K	1282.68	Joback Method
hsubt	140.00	kJ/mol	358.50	NIST Webbook

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=C28930292&Units=SI&Mask=3FFF

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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