Benzenamine, N-methyl-2,4-dinitro-

Other names: Aniline, N-methyl-2,4-dinitro-
N-Methyl-2,4-dinitroaniline
2,4-Dinitro-N-methylaniline
(2,4-Dinitrophenyl)methylamine
Inchi: InChI=1S/C7H7N3O4/c1-8-6-3-2-5(9(11)12)4-7(6)10(13)14/h2-4,8H,1H3
InchiKey: IQEJEZOCXWJNKR-UHFFFAOYSA-N
Formula: C7H7N3O4
SMILES: CNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 197.15
CAS: 2044-88-4

Physical Properties

Property code	Value	Unit	Source
chs	-3705.00	kJ/mol	NIST Webbook
chs	-3688.00 ± 3.70	kJ/mol	NIST Webbook
gf	261.70	kJ/mol	Joback Method
hf	57.73	kJ/mol	Joback Method
hfs	-67.40 ± 3.70	kJ/mol	NIST Webbook
hfus	34.97	kJ/mol	Joback Method
hvap	74.39	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	1.545		Crippen Method
mcvol	130.550	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
tb	750.05	K	Joback Method
tc	1018.88	K	Joback Method
tf	559.99	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.20	J/mol×K	750.05	Joback Method
cpg	352.67	J/mol×K	794.86	Joback Method

cpg	361.22	J/mol×K	839.66	Joback Method
cpg	368.92	J/mol×K	884.47	Joback Method
cpg	375.82	J/mol×K	929.27	Joback Method
cpg	381.97	J/mol×K	974.08	Joback Method
cpg	387.43	J/mol×K	1018.88	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=C2044884&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume