Methanediamine, N,N'-dimethyl-N,N'-dinitro-

Inchi: InChI=1S/C3H8N4O4/c1-4(6(8)9)3-5(2)7(10)11/h3H2,1-2H3
InchiKey: QKVCTKJCIMPZEI-UHFFFAOYSA-N
Formula: C3H8N4O4
SMILES: CN(CN(C)[N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 164.12
CAS: 13232-00-3

Physical Properties

Property code	Value	Unit	Source
gf	267.04	kJ/mol	Joback Method
hf	8.29	kJ/mol	Joback Method
hfs	-36.60	kJ/mol	NIST Webbook
hfs	-29.80 ± 2.30	kJ/mol	NIST Webbook
hfus	32.29	kJ/mol	Joback Method
hvap	59.54	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	-0.809		Crippen Method
mcvol	107.930	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
tb	596.60	K	Joback Method
tc	830.82	K	Joback Method
tf	475.73	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.08	J/mol×K	791.78	Joback Method
cpg	272.39	J/mol×K	596.60	Joback Method
cpg	282.19	J/mol×K	635.64	Joback Method
cpg	291.21	J/mol×K	674.67	Joback Method
cpg	299.50	J/mol×K	713.71	Joback Method
cpg	307.11	J/mol×K	752.75	Joback Method
cpg	320.47	J/mol×K	830.82	Joback Method

hfust	16.36	kJ/mol	330.20	NIST Webbook

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=C13232003&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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion 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