N,N'-Dimethyl-N,N'-dinitro-ethanediamide

Other names: Ethanediamide, N,N'-dimethyl-N,N'-dinitro-
Oxamide, N,N'-dimethyl-N'-dinitro-
Ethanediamide, N',N''-dimethyl-N',N''-dinitro-
Inchi: InChI=1S/C4H6N4O6/c1-5(7(11)12)3(9)4(10)6(2)8(13)14/h1-2H3
InchiKey: DHNCWGKMISNJQG-UHFFFAOYSA-N
Formula: C4H6N4O6
SMILES: CN(C(=O)C(=O)N(C)[N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 206.11
CAS: 14760-99-7

Physical Properties

Property code	Value	Unit	Source
chs	-2126.20	kJ/mol	NIST Webbook
gf	17.62	kJ/mol	Joback Method
hf	-237.51	kJ/mol	Joback Method
hfs	-305.30	kJ/mol	NIST Webbook
hfus	38.08	kJ/mol	Joback Method
hvap	75.26	kJ/mol	Joback Method
log10ws	-0.34		Crippen Method
logp	-1.713		Crippen Method
mcvol	125.160	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
tb	727.22	K	Joback Method
tc	968.71	K	Joback Method
tf	586.86	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.01	J/mol×K	727.22	Joback Method
cpg	340.74	J/mol×K	767.47	Joback Method
cpg	347.72	J/mol×K	807.72	Joback Method
cpg	353.99	J/mol×K	847.97	Joback Method

cpg	359.61	J/mol×K	888.22	Joback Method
cpg	364.64	J/mol×K	928.47	Joback Method
cpg	369.11	J/mol×K	968.71	Joback Method
hfust	23.40	kJ/mol	397.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14760997&Units=SI
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

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
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