

# Ethene-1,1-diamine, 2,2-dinitro-

Other names:	1,1-Ethenediamine, 2,2-dinitro- 1,1-diamino-2,2-dinitroethene 1,1-diamino-2,2-dinitroethylene DADNE DADNE (1,1-diamino-2,2-dinitroethene) FOX-7 FOX-7 (1,1-diamino-2,2-dinitroethene)
Inchi:	InChI=1S/C2H4N4O4/c3-1(4)2(5(7)8)6(9)10/h3-4H2
InchiKey:	FUHQFAMVYDIUKL-UHFFFAOYSA-N
Formula:	C2H4N4O4
SMILES:	NC(N)=C([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]:	148.08
CAS:	145250-81-3

## Physical Properties

Property code	Value	Unit	Source
gf	233.08	kJ/mol	Joback Method
hf	59.09	kJ/mol	Joback Method
hfus	31.63	kJ/mol	Joback Method
hvap	74.63	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	-1.416		Crippen Method
mcvol	89.540	ml/mol	McGowan Method
pc	6830.13	kPa	Joback Method
tb	697.82	K	Joback Method
tc	979.52	K	Joback Method
tf	533.04	K	Joback Method
tt	393.70	K	Comment on Studies on Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Derivatives
vc	0.351	m3/kmol	

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.18	J/molxK	979.52	Joback Method
cpg	250.32	J/molxK	932.57	Joback Method
cpg	246.17	J/molxK	885.62	Joback Method
cpg	241.65	J/molxK	838.67	Joback Method
cpg	236.68	J/molxK	791.72	Joback Method
cpg	231.17	J/molxK	744.77	Joback Method
cpg	225.07	J/molxK	697.82	Joback Method
cps	176.51	J/molxK	298.00	Studies on Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Derivatives
cps	201.68	J/molxK	353.00	Studies on Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Derivatives
cps	197.09	J/molxK	343.00	Studies on Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Derivatives
cps	192.50	J/molxK	333.00	Studies on Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Derivatives
cps	187.91	J/molxK	323.00	Studies on Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Derivatives
cps	183.32	J/molxK	313.00	Studies on Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Derivatives
cps	178.73	J/molxK	303.00	Studies on Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Derivatives

cps	174.14	J/molxK	293.00	Studies on Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Derivatives
cps	169.55	J/molxK	283.00	Studies on Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Derivatives

## Sources

Solubility of 1,1-diamino-2,2-dinitroethylene in different solvents and binary mixtures (1,1-diamino-2,2-dinitroethylene-water) and (N,N-dimethylformamide-pure ethyl sulfide and N-methyl-2-pyrrolidone: Comment on Studies on Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Derivatives : McGowan's Method:	<a href="https://www.doi.org/10.1016/j.fluid.2017.12.035">https://www.doi.org/10.1016/j.fluid.2017.12.035</a>
Crippen Method:	<a href="https://www.doi.org/10.1021/je900235s">https://www.doi.org/10.1021/je900235s</a>
Joback Method:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C145250813&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C145250813&amp;Units=SI</a>
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	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307i">http://pubs.acs.org/doi/abs/10.1021/ci990307i</a>
	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>cps:</b>	Solid phase heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume

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