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	Joback Method

Temperature Dependent Properties

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

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Comment on Studies on Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Derivatives :	https://www.doi.org/10.1021/acs.jced.6b00483
Studies on Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Derivatives:	https://www.doi.org/10.1021/acs.jced.5b00021
Solubility of 1,1-Diamino-2,2-dinitroethylene in N,N-Dimethylformamide, Dimethyl Sulfoxide, and N-Methyl-2-pyrrolidone:	https://www.doi.org/10.1021/je900235s
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of 1,1-diamino-2,2-dinitroethylene in different pure solvents and binary mixtures (dimethyl sulfoxide p water) and (N,N-dimethylformamide p water) at different temperatures:	https://www.doi.org/10.1016/j.fluid.2017.12.035
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C145250813&Units=SI

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
tt:	Triple Point Temperature
vc:	Critical Volume