Ethanol, 2,2'-oxybis-, dinitrate

Other names:	Diethylene glycol, dinitrate
	Diglycol dinitrate
	Dinitrodiglycol
	Oxydiethylene nitrate
	2,2'-Oxydiethanol dinitrate
	Digol dinitrate
	Bis(hydroxyaethyl)-aether-dinitrat
	Diethylenglykoldinitrate
	Diglycoldinitraat
	Diglykoldinitrat
	Di(hydroxyethyl) ether dinitrate
	Dinitrate de diethylene-glycol
	Dinitrodiglicol
	Dinitrodiglykol
	DEGDN
	Ethanol, 2,2'-oxybis-, 1,1'-dinitrate
	oxydiethylene dinitrate
Inchi:	InChI=1S/C4H8N2O7/c7-5(8)12-3-1-11-2-4-13-6(9)10/h1-4H2
InchiKey:	LYAGTVMJGHTIDH-UHFFFAOYSA-N
Formula:	C4H8N2O7
SMILES:	O=[N+]([O-])OCCOCCO[N+](=O)[O-]
Mol. weight [g/mol]:	196.12
CAS:	693-21-0

Physical Properties

Property code	Value	Unit	Source
chl	-2261.00	kJ/mol	NIST Webbook
chl	-2291.00	kJ/mol	NIST Webbook
chl	-2297.60	kJ/mol	NIST Webbook
chl	-2291.00	kJ/mol	NIST Webbook
gf	-261.10	kJ/mol	Joback Method
hf	-544.07	kJ/mol	Joback Method
hfl	-451.00	kJ/mol	NIST Webbook
hfs	-476.10	kJ/mol	NIST Webbook
hfus	32.40	kJ/mol	Joback Method
hvap	64.91	kJ/mol	Joback Method
log10ws	-0.91		Crippen Method

logp	-0.580		Crippen Method
mcvol	119.670	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
rinpol	1351.13		NIST Webbook
rinpol	1357.28		NIST Webbook
rinpol	1332.85		NIST Webbook
rinpol	1344.19		NIST Webbook
tb	661.86	K	Joback Method
tc	889.13	K	Joback Method
tf	488.75	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.11	J/mol×K	813.37	Joback Method
cpg	353.93	J/mol×K	851.25	Joback Method
cpg	313.45	J/mol×K	661.86	Joback Method
cpg	322.77	J/mol×K	699.74	Joback Method
cpg	331.51	J/mol×K	737.62	Joback Method
cpg	339.63	J/mol×K	775.49	Joback Method
cpg	360.04	J/mol×K	889.13	Joback Method
hfust	25.40	kJ/mol	276.50	NIST Webbook
hvapt	94.30	kJ/mol	313.00	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C693210&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume