1,2-Ethanediol, dinitrate

Other names:	1,2-Ethanediol, dinitrate
	Ethylene dinitrate
	Ethylene nitrate
	EGDN
	Glycol dinitrate
	Nitroglycol
	Dinitroglicol
	Dinitroglycol
	Ethanediol dinitrate
	Ethylenglykoldinitrat
	Glycoldinitraat
	Glykoldinitrat
	Nitroglykol
	1,2-Ethanediol, 1,2-dinitrate
Inchi:	InChI=1S/C2H4N2O6/c5-3(6)9-1-2-10-4(7)8/h1-2H2
InchiKey:	UQXKXGWGFRWILX-UHFFFAOYSA-N
Formula:	C2H4N2O6
SMILES:	O=[N+]([O-])OCCO[N+](=O)[O-]
Mol. weight [g/mol]:	152.06

Physical Properties

Property code	Value	Unit	Source
chl	-1123.30	kJ/mol	NIST Webbook
hf	-191.19	kJ/mol	Cheméo Relay (1.0)
hfl	-233.00	kJ/mol	NIST Webbook
hfus	26.03	kJ/mol	Joback Method
hsub	103.80	kJ/mol	NIST Webbook
hvap	70.50	kJ/mol	NIST Webbook
ie	11.23	eV	Cheméo Relay (1.0)
log10ws	-1.51		Cheméo Relay (1.0)
logp	-0.597		Crippen Method
mcvol	85.620	ml/mol	McGowan Method
rinpol	1034.50		NIST Webbook
rinpol	1050.99		NIST Webbook
rinpol	1032.05		NIST Webbook
rinpol	1039.73		NIST Webbook
rinpol	1032.05		NIST Webbook

rinpol	1034.50		NIST Webbook
tb	444.70	K	Cheméo Relay (1.0)
tf	281.19	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.03	J/mol×K	713.74	Joback Method
cpg	202.05	J/mol×K	593.68	Joback Method
cpg	209.13	J/mol×K	633.70	Joback Method
cpg	215.80	J/mol×K	673.72	Joback Method
cpg	227.81	J/mol×K	753.75	Joback Method
cpg	233.11	J/mol×K	793.77	Joback Method
cpg	237.90	J/mol×K	833.79	Joback Method
hsubt	105.10	kJ/mol	358.50	NIST Webbook
hsubt	105.40	kJ/mol	369.00	NIST Webbook
hvapt	68.30	kJ/mol	269.00	NIST Webbook
hvapt	62.30 ± 0.40	kJ/mol	334.00	NIST Webbook
hvapt	68.60 ± 0.40	kJ/mol	308.00	NIST Webbook
hvapt	55.30	kJ/mol	404.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C628966&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity

hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point