

Ethylene glycol, 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
CAS:	628-96-6

Physical Properties

Property code	Value	Unit	Source
chl	-1123.30	kJ/mol	NIST Webbook
gf	-172.94	kJ/mol	Joback Method
hf	-370.57	kJ/mol	Joback Method
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
log10ws	-0.98		Crippen Method
logp	-0.597		Crippen Method
mcvol	85.620	ml/mol	McGowan Method
pc	4959.33	kPa	Joback Method
rinpol	1032.05		NIST Webbook
rinpol	1034.50		NIST Webbook
rinpol	1032.05		NIST Webbook

rinpol	1039.73		NIST Webbook
rinpol	1050.99		NIST Webbook
rinpol	1034.50		NIST Webbook
tb	593.68	K	Joback Method
tc	833.79	K	Joback Method
tf	443.98	K	Joback Method
vc	0.347	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C628966&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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
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
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

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