

Ethanol, 2-nitro-, nitrate (ester)

Other names:	2-Nitroethyl nitrate Ethanol, 2-nitro-, nitrate Nitroethyl nitrate
Inchi:	InChI=1S/C2H4N2O5/c5-3(6)1-2-9-4(7)8/h1-2H2
InchiKey:	FRXFYZJACNONHT-UHFFFAOYSA-N
Formula:	C2H4N2O5
SMILES:	O=[N+](([O-])CCO[N+](=O)[O-])
Mol. weight [g/mol]:	136.06
CAS:	4528-34-1

Physical Properties

Property code	Value	Unit	Source
chl	-927.17	kJ/mol	NIST Webbook
gf	-67.94	kJ/mol	Joback Method
hf	-238.35	kJ/mol	Joback Method
hfus	24.85	kJ/mol	Joback Method
hvap	55.64	kJ/mol	Joback Method
log10ws	-0.91		Crippen Method
logp	-0.529		Crippen Method
mcvol	79.750	ml/mol	McGowan Method
pc	5080.25	kPa	Joback Method
tb	571.26	K	Joback Method
tc	815.08	K	Joback Method
tf	421.75	K	Joback Method
vc	0.330	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.51	J/molxK	571.26	Joback Method
cpg	189.49	J/molxK	611.90	Joback Method
cpg	196.03	J/molxK	652.53	Joback Method
cpg	202.11	J/molxK	693.17	Joback Method
cpg	207.75	J/molxK	733.80	Joback Method

cpg	212.93	J/mol×K	774.44	Joback Method
cpg	217.67	J/mol×K	815.08	Joback Method

Sources

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=C4528341&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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
vc:	Critical Volume

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