Acetic acid, nitro-, ethyl ester

Other names:	Ethyl nitroacetate
	Nitroacetic acid ethyl ester
Inchi:	InChI=1S/C4H7NO4/c1-2-9-4(6)3-5(7)8/h2-3H2,1H3
InchiKey:	FTKASJMIPSSXBP-UHFFFAOYSA-N
Formula:	C4H7NO4
SMILES:	CCOC(=O)C[N+](=O)[O-]
Mol. weight [g/mol]:	133.10
CAS:	626-35-7

Physical Properties

Property code	Value	Unit	Source
chl	-2087.00 ± 1.50	kJ/mol	NIST Webbook
gf	-215.57	kJ/mol	Joback Method
hf	-381.45	kJ/mol	Joback Method
hfl	-487.00 ± 1.50	kJ/mol	NIST Webbook
hfus	20.26	kJ/mol	Joback Method
hvap	50.25	kJ/mol	Joback Method
log10ws	-0.44		Crippen Method
logp	-0.174		Crippen Method
mcvol	92.080	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
tb	519.05	K	Joback Method
tc	734.66	K	Joback Method
tf	350.61	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.60	J/mol×K	519.05	Joback Method
cpg	209.95	J/mol×K	554.99	Joback Method
cpg	217.90	J/mol×K	590.92	Joback Method
cpg	225.44	J/mol×K	626.86	Joback Method
cpg	232.58	J/mol×K	662.79	Joback Method

cpg	239.31	J/mol×K	698.73	Joback Method
cpg	245.63	J/mol×K	734.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.20	K	3.30	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=C626357&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
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume