Pentanoic acid, 4-methyl-4-nitro-, methyl ester

Other names:	Valeric acid, 4-methyl-4-nitro-, methyl ester
	Methyl 4-methyl-4-nitropentanoate
	Methyl 4-nitro-4-valerate
Inchi:	InChI=1S/C7H13NO4/c1-7(2,8(10)11)5-4-6(9)12-3/h4-5H2,1-3H3
InchiKey:	MROVMGGCWUQHMR-UHFFFAOYSA-N
Formula:	C7H13NO4
SMILES:	COC(=O)CCC(C)(C)[N+](=O)[O-]
Mol. weight [g/mol]:	175.18
CAS:	16507-02-1

Physical Properties

Property code	Value	Unit	Source
gf	-187.47	kJ/mol	Joback Method
hf	-452.12	kJ/mol	Joback Method
hfus	20.62	kJ/mol	Joback Method
hvap	55.63	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	0.995		Crippen Method
mcvol	134.350	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
tb	584.46	K	Joback Method
tc	802.30	K	Joback Method
tf	386.84	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.46	J/mol×K	584.46	Joback Method
cpg	348.67	J/mol×K	620.77	Joback Method
cpg	360.11	J/mol×K	657.07	Joback Method
cpg	370.81	J/mol×K	693.38	Joback Method
cpg	380.80	J/mol×K	729.69	Joback Method
cpg	390.11	J/mol×K	766.00	Joback Method

cpg	398.77	J/mol×K	802.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16507021&Units=SI
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

Legend

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