Propane, 2-nitro-2-nitroso-

Inchi: InChI=1S/C3H6N2O3/c1-3(2,4-6)5(7)8/h1-2H3
InchiKey: MYRROMXOABKDLG-UHFFFAOYSA-N
Formula: C3H6N2O3
SMILES: CC(C)(N=O)[N+](=O)[O-]
Mol. weight [g/mol]: 118.09
CAS: 5275-46-7

Physical Properties

Property code	Value	Unit	Source
hf	-292.95	kJ/mol	Joback Method
hvap	46.66	kJ/mol	Joback Method
ie	9.90 ± 0.10	eV	NIST Webbook
log10ws	-1.96		Crippen Method
logp	0.766		Crippen Method
mcvol	82.100	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	480.05	K	Joback Method
tc	701.58	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5275467&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

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
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