1-Propene, 3-nitro-

Inchi: InChI=1S/C3H5NO2/c1-2-3-4(5)6/h2H,1,3H2
InchiKey: VLISOFDTMSFZPP-UHFFFAOYSA-N
Formula: C3H5NO2
SMILES: C=CC[N+](=O)[O-]
Mol. weight [g/mol]: 87.08
CAS: 625-46-7

Physical Properties

Property code	Value	Unit	Source
gf	97.77	kJ/mol	Joback Method
hf	9.42	kJ/mol	Joback Method
hfus	13.61	kJ/mol	Joback Method
hvap	38.19	kJ/mol	Joback Method
ie	10.40	eV	NIST Webbook
ie	10.65	eV	NIST Webbook
log10ws	-1.02		Crippen Method
logp	0.449		Crippen Method
mcvol	66.250	ml/mol	McGowan Method
pc	4743.15	kPa	Joback Method
tb	400.70	K	NIST Webbook
tc	630.93	K	Joback Method
tf	265.42	K	Joback Method
vc	0.267	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.71	J/mol×K	416.56	Joback Method
cpg	125.65	J/mol×K	452.29	Joback Method
cpg	132.18	J/mol×K	488.02	Joback Method
cpg	138.32	J/mol×K	523.75	Joback Method
cpg	144.10	J/mol×K	559.48	Joback Method
cpg	149.53	J/mol×K	595.20	Joback Method
cpg	154.62	J/mol×K	630.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C625467&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
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
tf:	Normal melting (fusion) point
vc:	Critical Volume