Propane, 2-methyl-2-nitro-

Other names:	(CH3)3CNO2
	1,1-Dimethyl-1-nitroethane
	2-Methyl-2-nitropropane
	2-Nitro-2-methylpropane
	2-Nitroisobutane
	Trimethylnitromethane
	nitro-tert-butane
	tert-Nitrobutane
Inchi:	InChI=1S/C4H9NO2/c1-4(2,3)5(6)7/h1-3H3
InchiKey:	AIMREYQYBFBEGQ-UHFFFAOYSA-N
Formula:	C4H9NO2
SMILES:	CC(C)(C)[N+](=O)[O-]
Mol. weight [g/mol]:	103.12
CAS:	594-70-7

Physical Properties

Property code	Value	Unit	Source
chs	-2630.00 ± 3.00	kJ/mol	NIST Webbook
gf	21.19	kJ/mol	Joback Method
hf	-177.10 ± 3.30	kJ/mol	NIST Webbook
hfs	-230.00 ± 3.00	kJ/mol	NIST Webbook
hfus	10.06	kJ/mol	Joback Method
hvap	39.79	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.062		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
tb	399.00 ± 3.00	K	NIST Webbook
tb	400.31 ± 0.06	K	NIST Webbook
tb	400.65 ± 0.15	K	NIST Webbook
tb	400.50 ± 0.50	K	NIST Webbook
tb	400.40	K	NIST Webbook
tc	661.08	K	Joback Method
tf	298.65 ± 1.50	K	NIST Webbook
tf	299.38 ± 0.06	K	NIST Webbook
vc	0.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.05	J/mol×K	439.53	Joback Method
cpg	183.50	J/mol×K	476.46	Joback Method
cpg	193.24	J/mol×K	513.38	Joback Method
cpg	202.31	J/mol×K	550.31	Joback Method
cpg	210.74	J/mol×K	587.23	Joback Method
cpg	218.57	J/mol×K	624.16	Joback Method
cpg	225.85	J/mol×K	661.08	Joback Method
hfust	2.60	kJ/mol	299.20	NIST Webbook
hvapt	39.10	kJ/mol	367.50	NIST Webbook
pvap	2.05	kPa	299.30	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	2.55	kPa	303.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	2.71	kPa	304.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	3.26	kPa	308.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	3.53	kPa	309.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	4.21	kPa	313.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	4.41	kPa	314.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	5.27	kPa	318.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	6.65	kPa	323.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	8.48	kPa	328.10	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods	

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48963e+01
Coeff. B	-3.57637e+03
Coeff. C	-5.24360e+01
Temperature range (K), min.	297.25
Temperature range (K), max.	425.56

Sources

Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods:	https://www.doi.org/10.1016/j.tca.2017.07.001
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=C594707&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume