Propane, 2-methyl-1-nitro-

Other names:	(CH3)2CHCH2NO2
	1-Nitro-2-methylpropane
	1-Nitroisobutane
	2-Methyl-1-nitropropane
	2-Methyl-3-nitropropane
Inchi:	InChI=1S/C4H9NO2/c1-4(2)3-5(6)7/h4H,3H2,1-2H3
InchiKey:	XFXRMDNWSGXSNJ-UHFFFAOYSA-N
Formula:	C4H9NO2
SMILES:	CC(C)C[N+](=O)[O-]
Mol. weight [g/mol]:	103.12
CAS:	625-74-1

Physical Properties

Property code	Value	Unit	Source
gf	15.91	kJ/mol	Joback Method
hf	-141.93	kJ/mol	Joback Method
hfus	13.95	kJ/mol	Joback Method
hvap	40.70	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	0.919		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
rinpol	776.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	774.00		NIST Webbook
tb	414.87 ± 0.06	K	NIST Webbook
tc	654.36	K	Joback Method
tf	196.30 ± 0.06	K	NIST Webbook
vc	0.336	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.34	J/mol×K	442.32	Joback Method
cpg	179.92	J/mol×K	477.66	Joback Method
cpg	189.01	J/mol×K	513.00	Joback Method
cpg	197.63	J/mol×K	548.34	Joback Method
cpg	205.79	J/mol×K	583.68	Joback Method
cpg	213.51	J/mol×K	619.02	Joback Method
cpg	220.79	J/mol×K	654.36	Joback Method
hvapt	41.10	kJ/mol	381.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49334e+01
Coeff. B	-3.69678e+03
Coeff. C	-5.64840e+01
Temperature range (K), min.	308.90
Temperature range (K), max.	440.69

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C625741&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

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume