Propanamide, N-methyl-

Other names:	N-Methylpropanamide
	N-Methylpropionamide
	N-Methylpropionic acid amide
	N-Methylpropionsaureamid
	Propionamide, N-methyl-
Inchi:	InChI=1S/C4H9NO/c1-3-4(6)5-2/h3H2,1-2H3,(H,5,6)
InchiKey:	QJQAMHYHNCADNR-UHFFFAOYSA-N
Formula:	C4H9NO
SMILES:	CCC(=O)NC
Mol. weight [g/mol]:	87.12
CAS:	1187-58-2

Physical Properties

Property code	Value	Unit	Source
affp	920.40	kJ/mol	NIST Webbook
basg	864.00 ± 5.00	kJ/mol	NIST Webbook
basg	889.40	kJ/mol	NIST Webbook
chl	-2539.70 ± 0.80	kJ/mol	NIST Webbook
gf	-56.73	kJ/mol	Joback Method
hf	-185.00	kJ/mol	Joback Method
hfl	-320.10 ± 0.80	kJ/mol	NIST Webbook
hfus	12.81	kJ/mol	Joback Method
hvap	66.60 ± 0.20	kJ/mol	NIST Webbook
hvap	64.90 ± 0.30	kJ/mol	NIST Webbook
hvap	66.90 ± 1.30	kJ/mol	NIST Webbook
log10ws	-0.46		Crippen Method
logp	0.142		Crippen Method
mcvol	78.770	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
rinpol	897.00		NIST Webbook
rinpol	921.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1690.00		NIST Webbook
tb	394.96	K	Joback Method
tc	579.58	K	Joback Method
tf	237.43	K	Joback Method
vc	0.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	143.48	J/mol×K	394.96	Joback Method
cpg	151.71	J/mol×K	425.73	Joback Method
cpg	159.61	J/mol×K	456.50	Joback Method
cpg	167.19	J/mol×K	487.27	Joback Method
cpg	174.45	J/mol×K	518.04	Joback Method
cpg	181.39	J/mol×K	548.81	Joback Method
cpg	188.03	J/mol×K	579.58	Joback Method
cpl	179.00	J/mol×K	298.15	NIST Webbook
hvapt	64.00 ± 0.20	kJ/mol	339.00	NIST Webbook
hvapt	64.00 ± 0.30	kJ/mol	420.50	NIST Webbook
hvapt	54.20	kJ/mol	387.50	NIST Webbook
hvapt	54.40	kJ/mol	333.00	NIST Webbook
hvapt	56.60 ± 0.20	kJ/mol	430.50	NIST Webbook
hvapt	63.90 ± 0.20	kJ/mol	430.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	419.20	K	12.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	9.49285e+00
Coeff. B	-8.02697e+02
Coeff. C	-2.69445e+02
Temperature range (K), min.	354.25
Temperature range (K), max.	461.42

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1187582&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

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume