Formamide, N-(1,1-dimethylethyl)-

Other names:	Formamide, N-tert-butyl-
	N-(1,1-dimethylethyl)formamide
	N-TERT-BUTYLFORAMIDE
	N-tert-Butylformamide
	tert-Butylformamide
Inchi:	InChI=1S/C5H11NO/c1-5(2,3)6-4-7/h4H,1-3H3,(H,6,7)
InchiKey:	SDLAKRCBYGZJRW-UHFFFAOYSA-N
Formula:	C5H11NO
SMILES:	CC(C)(C)NC=O
Mol. weight [g/mol]:	101.15
CAS:	2425-74-3

Physical Properties

Property code	Value	Unit	Source
gf	-16.07	kJ/mol	Joback Method
hf	-187.39	kJ/mol	Joback Method
hfus	8.68	kJ/mol	Joback Method
hvap	38.58	kJ/mol	Joback Method
log10ws	-0.99		Crippen Method
logp	0.531		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
rinpol	915.00		NIST Webbook
tb	475.00	K	NIST Webbook
tb	475.20	K	NIST Webbook
tc	599.61	K	Joback Method
tf	243.19	K	Joback Method
vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.82	J/mol×K	409.40	Joback Method
cpg	194.36	J/mol×K	441.10	Joback Method

cpg	204.32	J/mol×K	472.80	Joback Method
cpg	213.72	J/mol×K	504.51	Joback Method
cpg	222.58	J/mol×K	536.21	Joback Method
cpg	230.92	J/mol×K	567.91	Joback Method
cpg	238.78	J/mol×K	599.61	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.50 ± 0.50	K	3.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51603e+01
Coeff. B	-4.23692e+03
Coeff. C	-7.32420e+01
Temperature range (K), min.	358.12
Temperature range (K), max.	503.44

Sources

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

Critical Assessment of CO2 Solubility in Volatile Solvents at 298.15 K: https://www.doi.org/10.1021/je101161d

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol1384.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2425743&Units=SI

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume