Benzamide, N-methyl-

Other names:	N-methylbenzamide
	N-methylbenzenamide
Inchi:	InChI=1S/C8H9NO/c1-9-8(10)7-5-3-2-4-6-7/h2-6H,1H3,(H,9,10)
InchiKey:	NCCHARWOCKOHIH-UHFFFAOYSA-N
Formula:	C8H9NO
SMILES:	CNC(=O)c1ccccc1
Mol. weight [g/mol]:	135.16
CAS:	613-93-4

Physical Properties

Property code	Value	Unit	Source
gf	89.36	kJ/mol	Joback Method
hf	-31.03	kJ/mol	Joback Method
hfus	18.62	kJ/mol	Thermodynamic Study of Benzamide, N-Methylbenzamide, and N,N-Dimethylbenzamide: Vapor Pressures, Phase Diagrams, and Hydrogen Bond Enthalpy
hvap	48.86	kJ/mol	Joback Method
ie	9.33 ± 0.05	eV	NIST Webbook
log10ws	-1.82		Crippen Method
logp	1.046		Crippen Method
mcvol	111.370	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
rinpol	1390.00		NIST Webbook
rinpol	1404.00		NIST Webbook
tb	513.16	K	Joback Method
tc	735.85	K	Joback Method
tf	352.00 ± 3.00	K	NIST Webbook
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	234.64	J/mol×K	513.16	Joback Method
cpg	246.69	J/mol×K	550.28	Joback Method
cpg	257.95	J/mol×K	587.39	Joback Method
cpg	268.45	J/mol×K	624.51	Joback Method
cpg	278.21	J/mol×K	661.62	Joback Method
cpg	287.28	J/mol×K	698.74	Joback Method
cpg	295.69	J/mol×K	735.85	Joback Method
hsubt	75.00	kJ/mol	309.00	NIST Webbook
hsubt	85.70	kJ/mol	318.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	440.20	K	1.50	NIST Webbook
tbrp	437.50 ± 0.50	K	2.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C613934&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic Study of Benzamide, N-Methylbenzamide, and N,N-Dimethylbenzamide: Vapor Pressures, Phase Diagrams, and Hydrogen Bond Enthalpy:	https://www.doi.org/10.1021/je100175j
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hsubt:	Enthalpy of sublimation at a given temperature
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
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