Benzamide, N-phenyl-

Other names:	Benzoic acid anilide
	N-Benzoylaniline
	N-Phenylbenzoic acid amide
	N-phenylbenzamide
	benzamide, N-phenyl
	benzanilide
Inchi:	InChI=1S/C13H11NO/c15-13(11-7-3-1-4-8-11)14-12-9-5-2-6-10-12/h1-10H,(H,14,15)
InchiKey:	ZVSKZLHKADLHSD-UHFFFAOYSA-N
Formula:	C13H11NO
SMILES:	O=C(Nc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	197.23
CAS:	93-98-1

Physical Properties

Property code	Value	Unit	Source
gf	243.87	kJ/mol	Joback Method
hf	102.30	kJ/mol	Joback Method
hfus	31.20	kJ/mol	Vaporization and Sublimation Enthalpies of Acetanilide and Several Derivatives by Correlation Gas Chromatography
hsub	125.40 ± 2.30	kJ/mol	NIST Webbook
hvap	62.27	kJ/mol	Joback Method
ie	8.10 ± 0.10	eV	NIST Webbook
log10ws	-3.45		Crippen Method
logp	2.939		Crippen Method
mcvol	158.060	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
rinpol	1989.00		NIST Webbook
tb	654.24	K	Joback Method
tc	903.46	K	Joback Method
tf	433.00 ± 3.00	K	NIST Webbook
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.03	J/mol×K	654.24	Joback Method
cpg	405.57	J/mol×K	695.78	Joback Method
cpg	418.84	J/mol×K	737.31	Joback Method
cpg	430.93	J/mol×K	778.85	Joback Method
cpg	441.92	J/mol×K	820.39	Joback Method
cpg	451.90	J/mol×K	861.93	Joback Method
cpg	460.95	J/mol×K	903.46	Joback Method
hfust	29.61	kJ/mol	436.49	NIST Webbook
hfust	32.40	kJ/mol	436.30	NIST Webbook
hfust	29.61	kJ/mol	436.50	NIST Webbook
hfust	29.61	kJ/mol	436.50	NIST Webbook
hsubt	99.20	kJ/mol	360.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	390.20	K	1.30	NIST Webbook

Sources

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=C93981&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vaporization and Sublimation Enthalpies of Acetanilide and Several Derivatives by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je300152t

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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