Benzamide

Other names:	Benzoic acid amide
	Benzoylamide
	Phenylcarboxyamide
Inchi:	InChI=1S/C7H7NO/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H2,8,9)
InchiKey:	KXDAEFPNCMNJSK-UHFFFAOYSA-N
Formula:	C7H7NO
SMILES:	NC(=O)c1ccccc1
Mol. weight [g/mol]:	121.14
CAS:	55-21-0

Physical Properties

Property code	Value	Unit	Source
affp	892.10	kJ/mol	NIST Webbook
basg	861.20	kJ/mol	NIST Webbook
chs	-3550.10 ± 0.80	kJ/mol	NIST Webbook
chs	-3546.50 ± 1.90	kJ/mol	NIST Webbook
chs	-3552.20	kJ/mol	NIST Webbook
chs	-3551.00 ± 3.00	kJ/mol	NIST Webbook
chs	-3552.80 ± 0.50	kJ/mol	NIST Webbook
gf	58.00	kJ/mol	Joback Method
hf	-30.07	kJ/mol	Joback Method
hfs	-208.50 ± 1.90	kJ/mol	NIST Webbook
hfs	-204.80 ± 0.80	kJ/mol	NIST Webbook
hfs	-202.14 ± 0.60	kJ/mol	NIST Webbook
hfs	-202.80	kJ/mol	NIST Webbook
hfus	23.18	kJ/mol	Thermodynamic Study of Benzamide, N-Methylbenzamide, and N,N-Dimethylbenzamide: Vapor Pressures, Phase Diagrams, and Hydrogen Bond Enthalpy
hfus	84.40	kJ/mol	Validation of the Vaporization Enthalpies of Some Simple Aliphatic Amides and Their Use in the Evaluation of the Vaporization Enthalpy of Valpromide and Valnoctamide
hsub	102.00 ± 1.00	kJ/mol	NIST Webbook

hvap	50.84	kJ/mol	Joback Method
ie	9.40 ± 0.20	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
ie	9.45	eV	NIST Webbook
ie	9.25	eV	NIST Webbook
log10ws	-0.99		Aqueous Solubility Prediction Method
log10ws	-0.95		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-0.96		Estimated Solubility Method
logp	0.786		Crippen Method
mcvol	97.280	ml/mol	McGowan Method
pc	4829.24	kPa	Joback Method
rinpol	1344.00		NIST Webbook
rinpol	1339.00		NIST Webbook
tb	561.00	K	NIST Webbook
tc	749.85	K	Joback Method
tf	402.30 ± 0.20	K	NIST Webbook
tf	403.00 ± 2.00	K	NIST Webbook
tf	400.00 ± 2.00	K	NIST Webbook
tf	400.40 ± 0.20	K	NIST Webbook
tf	400.00 ± 1.50	K	NIST Webbook
tf	401.25	K	Aqueous Solubility Prediction Method
tf	403.00	K	NIST Webbook
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.16	J/mol×K	512.64	Joback Method
cpg	211.79	J/mol×K	552.18	Joback Method
cpg	221.64	J/mol×K	591.71	Joback Method
cpg	230.76	J/mol×K	631.25	Joback Method
cpg	239.17	J/mol×K	670.78	Joback Method
cpg	246.92	J/mol×K	710.32	Joback Method
cpg	254.04	J/mol×K	749.85	Joback Method
cps	153.80	J/mol×K	298.15	NIST Webbook
hfust	23.76	kJ/mol	403.00	NIST Webbook
hfust	19.15	kJ/mol	402.10	NIST Webbook
hfust	18.49	kJ/mol	402.30	NIST Webbook

hsubt	96.90	kJ/mol	333.50	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Partial molar volumes of some drug and pro-drug substances in 1-octanol at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2009.10.002
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55210&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Measurement and correlation of solubility of benzamide in supercritical carbon dioxide with and without cosolvent:	https://www.doi.org/10.1016/j.fluid.2011.04.021
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
Validation of the Vaporization Enthalpies of Some Simple Aliphatic Amides and Their Use in the Evaluation of the Vaporization Enthalpy of Valpromide and Valnoctamide:	https://www.doi.org/10.1021/je3012452
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume