Benzeneacetamide

Other names:	Acetamide, 2-phenyl- «alpha»-Phenylacetamide «alpha»-Toluamide Phenyl-«beta»-acetylamine Phenylacetic acid amide 2-Phenylacetamide Phenylacetamide
Inchi:	InChI=1S/C8H9NO/c9-8(10)6-7-4-2-1-3-5-7/h1-5H,6H2,(H2,9,10)
InchiKey:	LSBDFXRDZJMBSC-UHFFFAOYSA-N
Formula:	C8H9NO
SMILES:	NC(=O)Cc1ccccc1
Mol. weight [g/mol]:	135.16
CAS:	103-81-1

Physical Properties

Property code	Value	Unit	Source
chs	-4224.33	kJ/mol	NIST Webbook
chs	-4210.40 ± 3.80	kJ/mol	NIST Webbook
gf	66.42	kJ/mol	Joback Method
hf	-50.71	kJ/mol	Joback Method
hfs	-209.70	kJ/mol	NIST Webbook
hfs	-224.00 ± 3.80	kJ/mol	NIST Webbook
hfus	17.31	kJ/mol	Joback Method
hvap	53.06	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	0.714		Crippen Method
mcvol	111.370	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
rinpol	1411.90		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1411.90		NIST Webbook
ripol	2660.00		NIST Webbook
ripol	2650.00		NIST Webbook
ripol	2650.00		NIST Webbook
ripol	2660.00		NIST Webbook
tb	535.52	K	Joback Method
tc	768.22	K	Joback Method

tf	339.53	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.60	J/mol×K	535.52	Joback Method
cpg	255.36	J/mol×K	574.30	Joback Method
cpg	266.29	J/mol×K	613.09	Joback Method
cpg	276.43	J/mol×K	651.87	Joback Method
cpg	285.82	J/mol×K	690.65	Joback Method
cpg	294.50	J/mol×K	729.44	Joback Method
cpg	302.51	J/mol×K	768.22	Joback Method
hsubt	96.40	kJ/mol	340.50	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C103811&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas 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
hsubt: Enthalpy of sublimation at a given temperature
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume