Butanamide, 3-oxo-N-phenyl-

Other names:	Acetoacetamidobenzene
	Acetoacetanilide
	Acetoacetic acid anilide
	Acetoacetic anilide
	[(Acetoacetyl)amino]benzene
	Acetoacetylaniline
	«alpha»-Acetylacetanilide
	N-(Acetylacetyl)aniline
	«alpha»-Acetyl-N-phenylacetamide
	«beta»-Ketobutyranilide
	3-Oxo-N-phenylbutanamide
	N-Phenylacetoacetamide
	1-(Phenylcarbamoyl)-2-propanone
	Acetanilide, 2-acetyl-
	Acetylacetanilide
	USAF EK-1239
	AAN
	Acetoacetanilid
	Anilid kyseliny acetoctove
	Acetoacetonilide
	NSC 2656
Inchi:	InChI=1S/C10H11NO2/c1-8(12)7-10(13)11-9-5-3-2-4-6-9/h2-6H,7H2,1H3,(H,11,13)
InchiKey:	DYRDKSSFIWVSNM-UHFFFAOYSA-N
Formula:	C10H11NO2
SMILES:	CC(=O)CC(=O)Nc1ccccc1
Mol. weight [g/mol]:	177.20
CAS:	102-01-2

Physical Properties

Property code	Value	Unit	Source
gf	-22.72	kJ/mol	Joback Method
hf	-184.89	kJ/mol	Joback Method
hfus	23.99	kJ/mol	Joback Method
hvap	60.06	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.604		Crippen Method

mcvol	141.120	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
tb	612.79	K	Joback Method
tc	835.48	K	Joback Method
tf	381.40	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.59	J/mol×K	612.79	Joback Method
cpg	352.03	J/mol×K	649.91	Joback Method
cpg	363.59	J/mol×K	687.02	Joback Method
cpg	374.32	J/mol×K	724.14	Joback Method
cpg	384.24	J/mol×K	761.25	Joback Method
cpg	393.41	J/mol×K	798.37	Joback Method
cpg	401.86	J/mol×K	835.48	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C102012&Units=SI
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

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