Butanamide, N-(4-chlorophenyl)-3-oxo-

Other names:	Acetoacetanilide, 4'-chloro-
	p-Chloroacetoacetanilide
	Acetoacet-p-chloroanilide
	Acetoacetyl-4-chloroanilide
	4'-Chloroacetoacetanilide
	Acetoacetic acid-4-chloroanilide
	Acetoacetanilide, p-chloro-
	N-(4-Chlorophenyl)acetoacetamide
	Butanamide, 3-oxo-N-(4-chlorophenyl)-
	N-(4-Chloro-phenyl)-3-oxo-butyramide
	N-(4-Chlorophenyl)acetylacetamide
	NSC 3544
Inchi:	InChI=1S/C10H10ClNO2/c1-7(13)6-10(14)12-9-4-2-8(11)3-5-9/h2-5H,6H2,1H3,(H,12,14)
InchiKey:	JMRJWEJJUKUBEA-UHFFFAOYSA-N
Formula:	C10H10ClNO2
SMILES:	CC(=O)CC(=O)Nc1ccc(Cl)cc1
Mol. weight [g/mol]:	211.65
CAS:	101-92-8

Physical Properties

Property code	Value	Unit	Source
gf	-44.28	kJ/mol	Joback Method
hf	-212.10	kJ/mol	Joback Method
hfus	27.80	kJ/mol	Joback Method
hvap	65.11	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.258		Crippen Method
mcvol	153.360	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
tb	655.20	K	Joback Method
tc	882.11	K	Joback Method
tf	423.84	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.94	J/mol×K	655.20	Joback Method
cpg	373.15	J/mol×K	693.02	Joback Method
cpg	383.55	J/mol×K	730.84	Joback Method
cpg	393.15	J/mol×K	768.65	Joback Method
cpg	402.00	J/mol×K	806.47	Joback Method
cpg	410.14	J/mol×K	844.29	Joback Method
cpg	417.60	J/mol×K	882.11	Joback Method

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=C101928&Units=SI

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

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