p-Acetoacetanisidide

Other names:	Butanamide, N-(4-methoxyphenyl)-3-oxo- p-Acetoacetanisidine para-Acetoacetanisidide N-(4-Methoxyphenyl)acetoacetamide 4'-Methoxyacetoacetanilide Acetoacetanilide, 4'-methoxy- Acetoacet-p-anisidide Butanamide, N-(4-methoxyphenyl)-oxo- p-Methoxyacetoacetanilide N-(4-Methoxy-phenyl)-3-oxo-butyramide Butanamide, 3-oxo-N-(4-methoxyphenyl)- N-(4-Methoxyphenyl)acetylacetamide NSC 116392 NSC 16508 NSC 216130
Inchi:	InChI=1S/C11H13NO3/c1-8(13)7-11(14)12-9-3-5-10(15-2)6-4-9/h3-6H,7H2,1-2H3,(H,12,
InchiKey:	SWAJJKROCOJICG-UHFFFAOYSA-N
Formula:	C11H13NO3
SMILES:	COc1ccc(NC(=O)CC(C)=O)cc1
Mol. weight [g/mol]:	207.23
CAS:	5437-98-9

Physical Properties

Property code	Value	Unit	Source
gf	-128.93	kJ/mol	Joback Method
hf	-349.22	kJ/mol	Joback Method
hfus	27.38	kJ/mol	Joback Method
hvap	65.36	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.613		Crippen Method
mcvol	161.080	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
tb	663.07	K	Joback Method
tc	880.04	K	Joback Method
tf	427.42	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.36	J/mol×K	663.07	Joback Method
cpg	424.02	J/mol×K	699.23	Joback Method
cpg	435.84	J/mol×K	735.39	Joback Method
cpg	446.86	J/mol×K	771.56	Joback Method
cpg	457.08	J/mol×K	807.72	Joback Method
cpg	466.52	J/mol×K	843.88	Joback Method
cpg	475.19	J/mol×K	880.04	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=C5437989&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