4'-METHOXYACETOACETANILIDE

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

Physical Properties

Property code	Value	Unit	Source
hf	-411.61	kJ/mol	Cheméo Relay (1.0)
hfus	27.38	kJ/mol	Joback Method
hvap	79.87	kJ/mol	Cheméo Relay (1.0)
ie	7.61	eV	Cheméo Relay (1.0)
log10ws	-1.92		Cheméo Relay (1.0)
logp	1.613		Crippen Method
mcvol	161.080	ml/mol	McGowan Method
tb	603.97	K	Cheméo Relay (1.0)
tf	392.23	K	Cheméo Relay (1.0)

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: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5437989&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
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
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point