Benzoic acid, 4-(acetylamino)-, methyl ester

Other names:	Methyl 4-(acetylamino)benzoate
	Methyl N-acetylaminobenzoate
	methyl 4-acetamidobenzoate
Inchi:	InChI=1S/C10H11NO3/c1-7(12)11-9-5-3-8(4-6-9)10(13)14-2/h3-6H,1-2H3,(H,11,12)
InchiKey:	QKWTXJSLAZKYGV-UHFFFAOYSA-N
Formula:	C10H11NO3
SMILES:	COC(=O)c1ccc(NC(C)=O)cc1
Mol. weight [g/mol]:	193.20
CAS:	17012-22-5

Physical Properties

Property code	Value	Unit	Source
gf	-137.35	kJ/mol	Joback Method
hf	-328.58	kJ/mol	Joback Method
hfus	24.79	kJ/mol	Joback Method
hvap	63.13	kJ/mol	Joback Method
log10ws	-1.82		Aqueous Solubility Prediction Method
logp	1.432		Crippen Method
mcvol	146.990	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpol	1896.00		NIST Webbook
tb	640.19	K	Joback Method
tc	860.95	K	Joback Method
tf	416.15	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.17	J/mol×K	640.19	Joback Method
cpg	374.16	J/mol×K	676.98	Joback Method
cpg	385.36	J/mol×K	713.78	Joback Method
cpg	395.79	J/mol×K	750.57	Joback Method

cpg	405.45	J/mol×K	787.37	Joback Method
cpg	414.37	J/mol×K	824.16	Joback Method
cpg	422.55	J/mol×K	860.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17012225&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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