(3,4-Dimethoxy-benzoylamino)-acetic acid methyl ester

Other names: Glycin, N-(3,4-dimethoxybenzoyl), methyl ester
Inchi: InChI=1S/C12H15NO5/c1-16-9-5-4-8(6-10(9)17-2)12(15)13-7-11(14)18-3/h4-6H,7H2,1-3
InchiKey: FJKYJWSUSRUZHG-UHFFFAOYSA-N
Formula: C12H15NO5
SMILES: COC(=O)CNC(=O)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 253.25

Physical Properties

Property code	Value	Unit	Source
gf	-340.14	kJ/mol	Joback Method
hf	-645.77	kJ/mol	Joback Method
hfus	31.96	kJ/mol	Joback Method
hvap	73.06	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	0.607		Crippen Method
mcvol	186.910	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	2121.00		NIST Webbook
rinpol	2121.00		NIST Webbook
rinpol	2121.00		NIST Webbook
tb	735.77	K	Joback Method
tc	946.16	K	Joback Method
tf	495.67	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.68	J/mol×K	735.77	Joback Method
cpg	524.25	J/mol×K	770.83	Joback Method
cpg	535.96	J/mol×K	805.90	Joback Method
cpg	546.77	J/mol×K	840.96	Joback Method
cpg	556.69	J/mol×K	876.03	Joback Method
cpg	565.68	J/mol×K	911.09	Joback Method

cpg	573.73	J/mol×K	946.16	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=R106580&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume