

Glycine, N-(m-anisoyl)-, methyl ester

Other names:	(3-Methoxy-benzoylamino)-acetic acid methyl ester Glycin, N-(3-methoxybenzoyl), methyl ester
Inchi:	InChI=1S/C11H13NO4/c1-15-9-5-3-4-8(6-9)11(14)12-7-10(13)16-2/h3-6H,7H2,1-2H3,(H,
InchiKey:	BJTUNGVYWCBMKA-UHFFFAOYSA-N
Formula:	C11H13NO4
SMILES:	COC(=O)CNC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	223.23

Physical Properties

Property code	Value	Unit	Source
gf	-233.93	kJ/mol	Joback Method
hf	-481.44	kJ/mol	Joback Method
hfus	28.57	kJ/mol	Joback Method
hvap	67.77	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	0.598		Crippen Method
mcvol	166.950	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinpol	1893.00		NIST Webbook
rinpol	1922.00		NIST Webbook
rinpol	1893.00		NIST Webbook
rinpol	1922.00		NIST Webbook
tb	685.49	K	Joback Method
tc	900.03	K	Joback Method
tf	449.65	K	Joback Method
vc	0.626	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.99	J/molxK	685.49	Joback Method
cpg	448.41	J/molxK	721.25	Joback Method
cpg	460.02	J/molxK	757.00	Joback Method
cpg	470.80	J/molxK	792.76	Joback Method

cpg	480.77	J/mol×K	828.52	Joback Method
cpg	489.91	J/mol×K	864.28	Joback Method
cpg	498.24	J/mol×K	900.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299707&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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