GLYCINE, N-[(PHENYLMETHOXY)CARBONYL]-, METHYL ESTER

Other names: Carbobenzoxyglycine methyl ester
Glycine, N-[(phenylmethoxy)carbonyl]-, methyl ester
methyl N-benzyloxycarbonylglycinate

Inchi: InChI=1S/C11H13NO4/c1-15-10(13)7-12-11(14)16-8-9-5-3-2-4-6-9/h2-6H,7-8H2,1H3,(H,

InchiKey: DZYBBBYFLOPVOL-UHFFFAOYSA-N

Formula: C11H13NO4

SMILES: COC(=O)CNC(=O)OCc1ccccc1

Mol. weight [g/mol]: 223.23

Physical Properties

Property code	Value	Unit	Source
hfus	28.96	kJ/mol	Joback Method
hvap	88.28	kJ/mol	Cheméo Relay (1.0)
ie	9.11	eV	Cheméo Relay (1.0)
log10ws	-2.03		Cheméo Relay (1.0)
logp	1.086		Crippen Method
mcvol	166.950	ml/mol	McGowan Method
tb	573.71	K	Cheméo Relay (1.0)
tf	302.53	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.17	J/mol×K	680.51	Joback Method
cpg	449.74	J/mol×K	716.13	Joback Method
cpg	461.47	J/mol×K	751.74	Joback Method
cpg	472.35	J/mol×K	787.36	Joback Method
cpg	482.40	J/mol×K	822.98	Joback Method
cpg	491.62	J/mol×K	858.60	Joback Method
cpg	500.03	J/mol×K	894.21	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	430.00 ± 1.00	K	0.01	NIST Webbook

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=C1212539&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
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
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point