Carbobenzyloxyglycine 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
CAS: 1212-53-9

Physical Properties

Property code	Value	Unit	Source
gf	-224.30	kJ/mol	Joback Method
hf	-469.97	kJ/mol	Joback Method
hfus	28.96	kJ/mol	Joback Method
hvap	67.10	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.086		Crippen Method
mcvol	166.950	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
tb	680.51	K	Joback Method
tc	894.21	K	Joback Method
tf	437.13	K	Joback Method
vc	0.626	m3/kmol	Joback Method

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
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=C1212539&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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