

Glycine, N-(2-chlorobenzoyl)-, methyl ester

Inchi:	InChI=1S/C10H10ClNO3/c1-15-9(13)6-12-10(14)7-4-2-3-5-8(7)11/h2-5H,6H2,1H3,(H,12,
InchiKey:	NVWHFQJYAXGYIN-UHFFFAOYSA-N
Formula:	C10H10ClNO3
SMILES:	COC(=O)CNC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	227.64

Physical Properties

Property code	Value	Unit	Source
gf	-149.28	kJ/mol	Joback Method
hf	-344.32	kJ/mol	Joback Method
hfus	28.99	kJ/mol	Joback Method
hvap	67.52	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.243		Crippen Method
mvol	159.230	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	1782.00		NIST Webbook
rinpol	1782.00		NIST Webbook
tb	677.62	K	Joback Method
tc	901.54	K	Joback Method
tf	446.07	K	Joback Method
vc	0.602	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.28	J/mol×K	677.62	Joback Method
cpg	396.30	J/mol×K	714.94	Joback Method
cpg	406.52	J/mol×K	752.26	Joback Method
cpg	415.96	J/mol×K	789.58	Joback Method
cpg	424.64	J/mol×K	826.90	Joback Method
cpg	432.57	J/mol×K	864.22	Joback Method
cpg	439.76	J/mol×K	901.54	Joback Method

Sources

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=U299587&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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