

2-Amino-3-(3-chloro-4-methoxy-phenyl)propanoic acid, methyl ester

Other names:	Methyl 2-amino-3-(3-chloro-4-methoxyphenyl)propanoate
Inchi:	InChI=1S/C11H14ClNO3/c1-15-10-4-3-7(5-8(10)12)6-9(13)11(14)16-2/h3-5,9H,6,13H2,1
InchiKey:	QUBSTZJVDZUTFR-UHFFFAOYSA-N
Formula:	C11H14ClNO3
SMILES:	COC(=O)C(N)Cc1ccc(OC)c(Cl)c1
Mol. weight [g/mol]:	243.69

Physical Properties

Property code	Value	Unit	Source
gf	-151.95	kJ/mol	Joback Method
hf	-421.03	kJ/mol	Joback Method
hfus	27.36	kJ/mol	Joback Method
hvap	69.88	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	1.391		Crippen Method
mcvol	177.620	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	1900.00		NIST Webbook
rinpol	1900.00		NIST Webbook
tb	695.95	K	Joback Method
tc	919.68	K	Joback Method
tf	457.76	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.71	J/molxK	695.95	Joback Method
cpg	467.37	J/molxK	733.24	Joback Method
cpg	479.18	J/molxK	770.53	Joback Method
cpg	490.13	J/molxK	807.81	Joback Method
cpg	500.23	J/molxK	845.10	Joback Method
cpg	509.48	J/molxK	882.39	Joback Method
cpg	517.86	J/molxK	919.68	Joback Method

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=U378749&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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