

Benzoic acid, 3-amino-, methyl ester

Other names:	3-(methoxycarbonyl)aniline 3-aminobenzoic acid methyl ester 3-carbomethoxyaniline Methyl-3-aminobenzoate Methyl-m-aminobenzoate m-Aminobenzoic acid, methyl ester methyl 3-aminobenzoate methyl 3-aminophenylcarboxylate methyl m-aminobenzoate
Inchi:	InChI=1S/C8H9NO2/c1-11-8(10)6-3-2-4-7(9)5-6/h2-5H,9H2,1H3
InchiKey:	VZDNXXPBYLGWOS-UHFFFAOYSA-N
Formula:	C8NO2
SMILES:	COC(=O)c1cccc(N)c1
Mol. weight [g/mol]:	142.09
CAS:	4518-10-9

Physical Properties

Property code	Value	Unit	Source
gf	-48.21	kJ/mol	Joback Method
hf	-194.40	kJ/mol	Joback Method
hfus	17.80	kJ/mol	Thermodynamic study of phase transitions in methyl esters of ortho-, meta-, and para-aminobenzoic acids
hvap	56.14	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.055		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
rinpol	1475.00		NIST Webbook
tb	562.92	K	Joback Method
tc	793.64	K	Joback Method
tf	374.28	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.93	J/mol×K	562.92	Joback Method
cpg	276.15	J/mol×K	601.37	Joback Method
cpg	286.68	J/mol×K	639.83	Joback Method
cpg	296.53	J/mol×K	678.28	Joback Method
cpg	305.72	J/mol×K	716.73	Joback Method
cpg	314.25	J/mol×K	755.19	Joback Method
cpg	322.15	J/mol×K	793.64	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic study of phase transitions in methyl esters of ortho-, meta-, and para-aminobenzoic acids:	https://www.doi.org/10.1016/j.jct.2012.04.006
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=C4518109&Units=SI

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
mccvol:	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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