Benzoic acid, 3-amino-, ethyl ester

Other names:	3-(ethoxycarbonyl)aniline
	3-carbethoxyaniline
	3-ethoxycarbonylbenzeneamine
	Benzoic acid, m-amino-, ethyl ester
	ethyl 3-aminobenzoate
	ethyl m-aminobenzoate
	ethyl meta-aminobenzoate
	m-Aminobenzoic acid, ethyl ester
	m-ethoxycarbonylaniline
	meta-ethoxycarbonylaniline
Inchi:	InChI=1S/C9H11NO2/c1-2-12-9(11)7-4-3-5-8(10)6-7/h3-6H,2,10H2,1H3
InchiKey:	ZMCBYSBVJIMENC-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	CCOC(=O)c1cccc(N)c1
Mol. weight [g/mol]:	165.19
CAS:	582-33-2

Physical Properties

Property code	Value	Unit	Source
gf	-39.79	kJ/mol	Joback Method
hf	-215.04	kJ/mol	Joback Method
hfus	20.70	kJ/mol	Joback Method
hvap	58.36	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.446		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
tb	567.20	K	NIST Webbook
tb	567.00	K	NIST Webbook
tc	812.12	K	Joback Method
tf	385.55	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.15	J/mol×K	585.80	Joback Method
cpg	322.35	J/mol×K	623.52	Joback Method
cpg	333.81	J/mol×K	661.24	Joback Method
cpg	344.53	J/mol×K	698.96	Joback Method
cpg	354.54	J/mol×K	736.68	Joback Method
cpg	363.84	J/mol×K	774.40	Joback Method
cpg	372.45	J/mol×K	812.12	Joback Method
hvapt	83.18	kJ/mol	298.15	Thermal and structural properties of ethyl 2- and 3-aminobenzoates: Experimental and computational approaches

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	446.70	K	1.70	NIST Webbook
tbrp	417.00	K	0.70	NIST Webbook

Sources

Thermal and structural properties of ethyl 2- and 3-aminobenzoates: Experimental and computational approaches:	https://www.doi.org/10.1016/j.jct.2019.02.001
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=C582332&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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