ethyl anthranilate

Other names:	anthranilic acid, ethyl ester
	benzoic acid, 2-amino-, ethyl ester
	ethyl 2-aminobenzoate
	ethyl o-aminobenzoate
	o-aminobenzoic acid, ethyl ester
Inchi:	InChI=1S/C9H11NO2/c1-2-12-9(11)7-5-3-4-6-8(7)10/h3-6H,2,10H2,1H3
InchiKey:	TWLLPUMZVVGILS-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	CCOC(=O)c1ccccc1N
Mol. weight [g/mol]:	165.19
CAS:	87-25-2

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
rinpol	1387.00		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1452.00		NIST Webbook
ripol	2232.00		NIST Webbook
ripol	2232.00		NIST Webbook
ripol	2232.00		NIST Webbook
tb	540.00 ± 1.00	K	NIST Webbook
tb	541.20	K	NIST Webbook
tc	812.12	K	Joback Method

tf	287.50 ± 0.02	K	NIST Webbook
tf	286.00	K	NIST Webbook
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	70.95	kJ/mol	298.15	Thermal and structural properties of ethyl 2- and 3-aminobenzoates: Experimental and computational approaches
hvapt	59.60	kJ/mol	513.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	402.70	K	1.00	NIST Webbook
tbrp	419.20	K	2.00	NIST Webbook
tbrp	419.00 ± 1.00	K	2.00	NIST Webbook

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=C87252&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume