Ethyl 6-amino-3,4-dimethoxybenzoate

Other names: Benzoic acid, 2-amino-4,5-dimethoxy-, ethyl ester
ethyl 4,5-dimethoxyanthranilate
Inchi: InChI=1S/C11H15NO4/c1-4-16-11(13)7-5-9(14-2)10(15-3)6-8(7)12/h5-6H,4,12H2,1-3H3
InchiKey: SMICMEHDDWELMR-UHFFFAOYSA-N
Formula: C11H15NO4
SMILES: CCOC(=O)c1cc(OC)c(OC)cc1N
Mol. weight [g/mol]: 225.24
CAS: 20323-74-4

Physical Properties

Property code	Value	Unit	Source
gf	-252.21	kJ/mol	Joback Method
hf	-543.70	kJ/mol	Joback Method
hfus	27.48	kJ/mol	Joback Method
hvap	68.96	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.463		Crippen Method
mcvol	171.250	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
tb	686.36	K	Joback Method
tc	901.23	K	Joback Method
tf	477.59	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.46	J/mol×K	686.36	Joback Method
cpg	466.47	J/mol×K	722.17	Joback Method
cpg	478.71	J/mol×K	757.98	Joback Method
cpg	490.18	J/mol×K	793.80	Joback Method
cpg	500.83	J/mol×K	829.61	Joback Method
cpg	510.65	J/mol×K	865.42	Joback Method
cpg	519.62	J/mol×K	901.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20323744&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume