2-Amino-3,4,5-trimethoxybenzoic acid

Other names: Benzoic acid, 2-amino-3,4,5-trimethoxy-
3,4,5-trimethoxyanthranilic acid
Inchi: InChI=1S/C10H13NO5/c1-14-6-4-5(10(12)13)7(11)9(16-3)8(6)15-2/h4H,11H2,1-3H3,(H,1
InchiKey: JSHSRQCOCMIIPA-UHFFFAOYSA-N
Formula: C10H13NO5
SMILES: COc1cc(C(=O)O)c(N)c(OC)c1OC
Mol. weight [g/mol]: 227.21
CAS: 61948-85-4

Physical Properties

Property code	Value	Unit	Source
gf	-407.08	kJ/mol	Joback Method
hf	-686.76	kJ/mol	Joback Method
hfus	28.59	kJ/mol	Joback Method
hvap	84.07	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	0.993		Crippen Method
mcvol	163.030	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	760.64	K	Joback Method
tc	966.95	K	Joback Method
tf	539.66	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.22	J/mol×K	760.64	Joback Method
cpg	459.23	J/mol×K	795.03	Joback Method
cpg	468.56	J/mol×K	829.41	Joback Method
cpg	477.17	J/mol×K	863.80	Joback Method
cpg	485.04	J/mol×K	898.18	Joback Method
cpg	492.14	J/mol×K	932.57	Joback Method
cpg	498.44	J/mol×K	966.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61948854&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