1,3-Benzenedicarboxylic acid, 5-amino-, dimethyl ester

Other names: Isophthalic acid, 5-amino-, dimethyl ester
Dimethyl 5-aminoisophthalate
3,5-Dicarbomethoxyaniline
5-Aminoisophthalic acid dimethyl ester
5-Amino-1,3-isophthalic acid dimethyl ester

Inchi: InChI=1S/C10H11NO4/c1-14-9(12)6-3-7(10(13)15-2)5-8(11)4-6/h3-5H,11H2,1-2H3

InchiKey: DEKPYXUDJRABNK-UHFFFAOYSA-N

Formula: C10H11NO4

SMILES: COC(=O)c1cc(N)cc(C(=O)OC)c1

Mol. weight [g/mol]: 209.20

CAS: 99-27-4

Physical Properties

Property code	Value	Unit	Source
gf	-274.92	kJ/mol	Joback Method
hf	-491.95	kJ/mol	Joback Method
hfus	25.69	kJ/mol	Joback Method
hvap	70.41	kJ/mol	Joback Method
log10ws	-1.59		Crippen Method
logp	0.842		Crippen Method
mcvol	152.860	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
tb	689.95	K	Joback Method
tc	916.45	K	Joback Method
tf	481.50	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.39	J/mol×K	689.95	Joback Method
cpg	403.72	J/mol×K	727.70	Joback Method
cpg	414.26	J/mol×K	765.45	Joback Method
cpg	424.02	J/mol×K	803.20	Joback Method

cpg	432.97	J/mol×K	840.95	Joback Method
cpg	441.11	J/mol×K	878.70	Joback Method
cpg	448.43	J/mol×K	916.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99274&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

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