Methyl 2-(aminosulfonyl)benzoate

Other names:	2-Carbomethoxybenzenesulfonamide
	Benzoic acid, 2-(aminosulfonyl)-, methyl ester
	Benzoic acid, 2-sulfamoyl-, methyl ester
	2-Sulfamoylbenzoic acid methyl ester
	2-Carbomethoxybenzene sulphonamide
	methyl o-sulphamoylbenzoate
Inchi:	InChI=1S/C8H9NO4S/c1-13-8(10)6-4-2-3-5-7(6)14(9,11)12/h2-5H,1H3,(H2,9,11,12)
InchiKey:	VSOOBQALJVLTBH-UHFFFAOYSA-N
Formula:	C8H9NO4S
SMILES:	COC(=O)c1ccccc1S(N)(=O)=O
Mol. weight [g/mol]:	215.23
CAS:	57683-71-3

Physical Properties

Property code	Value	Unit	Source
gf	-516.75	kJ/mol	Joback Method
hf	-647.75	kJ/mol	Joback Method
hfus	29.49	kJ/mol	Joback Method
hvap	74.77	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	0.121		Crippen Method
mcvol	145.330	ml/mol	McGowan Method
pc	5015.69	kPa	Joback Method
tb	610.70	K	Joback Method
tc	831.78	K	Joback Method
tf	412.84	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.59	J/mol×K	610.70	Joback Method
cpg	354.05	J/mol×K	647.55	Joback Method
cpg	364.73	J/mol×K	684.39	Joback Method

cpg	374.63	J/mol×K	721.24	Joback Method
cpg	383.74	J/mol×K	758.09	Joback Method
cpg	392.05	J/mol×K	794.93	Joback Method
cpg	399.55	J/mol×K	831.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57683713&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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