

3-CH3SO2-C6H4-COOCH3

Inchi:	InChI=1S/C9H10O4S/c1-13-9(10)7-4-3-5-8(6-7)14(2,11)12/h3-6H,1-2H3
InchiKey:	QJLLSNKBORJJHO-UHFFFAOYSA-N
Formula:	C9H10O4S
SMILES:	COC(=O)c1cccc(S(C)(=O)=O)c1
Mol. weight [g/mol]:	214.24
CAS:	22821-69-8

Physical Properties

Property code	Value	Unit	Source
affp	830.50	kJ/mol	NIST Webbook
basg	799.50	kJ/mol	NIST Webbook
gf	-574.78	kJ/mol	Joback Method
hf	-702.18	kJ/mol	Joback Method
hfus	26.88	kJ/mol	Joback Method
hvap	66.36	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	0.877		Crippen Method
mcvol	149.440	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
tb	561.05	K	Joback Method
tc	770.42	K	Joback Method
tf	340.85	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.82	J/mol×K	561.05	Joback Method
cpg	346.41	J/mol×K	595.94	Joback Method
cpg	358.29	J/mol×K	630.84	Joback Method
cpg	369.46	J/mol×K	665.73	Joback Method
cpg	379.90	J/mol×K	700.63	Joback Method
cpg	389.62	J/mol×K	735.52	Joback Method
cpg	398.61	J/mol×K	770.42	Joback Method

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=C22821698&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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

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