4-SO2F-C6H4-COOCH3

Inchi: InChI=1S/C8H7FO4S/c1-13-8(10)6-2-4-7(5-3-6)14(9,11)12/h2-5H,1H3
InchiKey: ZHXUKAUTLJXSJX-UHFFFAOYSA-N
Formula: C8H7FO4S
SMILES: COC(=O)c1ccc(S(=O)(=O)F)cc1
Mol. weight [g/mol]: 218.20
CAS: 124397-38-2

Physical Properties

Property code	Value	Unit	Source
affp	802.60	kJ/mol	NIST Webbook
basg	771.60	kJ/mol	NIST Webbook
gf	-778.01	kJ/mol	Joback Method
hf	-877.65	kJ/mol	Joback Method
hfus	27.37	kJ/mol	Joback Method
hvap	63.31	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.131		Crippen Method
mcvol	137.120	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	537.44	K	Joback Method
tc	739.82	K	Joback Method
tf	330.17	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.18	J/mol×K	537.44	Joback Method
cpg	308.23	J/mol×K	571.17	Joback Method
cpg	318.69	J/mol×K	604.90	Joback Method
cpg	328.55	J/mol×K	638.63	Joback Method
cpg	337.81	J/mol×K	672.36	Joback Method
cpg	346.44	J/mol×K	706.09	Joback Method
cpg	354.45	J/mol×K	739.82	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=C124397382&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