3-Cl-4-CH3S-C6H3-COOCH3

Inchi: InChI=1S/C9H9ClO2S/c1-12-9(11)6-3-4-8(13-2)7(10)5-6/h3-5H,1-2H3
InchiKey: RKEOCHLSEHNYMF-UHFFFAOYSA-N
Formula: C9H9ClO2S
SMILES: COC(=O)c1ccc(SC)c(Cl)c1
Mol. weight [g/mol]: 216.69
CAS: 105442-23-7

Physical Properties

Property code	Value	Unit	Source
affp	856.30	kJ/mol	NIST Webbook
basg	825.40	kJ/mol	NIST Webbook
gf	-94.68	kJ/mol	Joback Method
hf	-234.17	kJ/mol	Joback Method
hfus	23.44	kJ/mol	Joback Method
hvap	59.59	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.849		Crippen Method
mcvol	149.940	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
tb	624.46	K	Joback Method
tc	866.16	K	Joback Method
tf	379.13	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.41	J/mol×K	624.46	Joback Method
cpg	336.78	J/mol×K	664.74	Joback Method
cpg	347.39	J/mol×K	705.03	Joback Method
cpg	357.23	J/mol×K	745.31	Joback Method
cpg	366.30	J/mol×K	785.59	Joback Method
cpg	374.59	J/mol×K	825.87	Joback Method
cpg	382.11	J/mol×K	866.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105442237&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

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