3-Cl-4-CH3S-C6H3-COCH3

Inchi: InChI=1S/C9H9ClOS/c1-6(11)7-3-4-9(12-2)8(10)5-7/h3-5H,1-2H3
InchiKey: IYWCQEVVYVUWFY-UHFFFAOYSA-N
Formula: C9H9ClOS
SMILES: CSc1ccc(C(C)=O)cc1Cl
Mol. weight [g/mol]: 200.69
CAS: 32467-66-6

Physical Properties

Property code	Value	Unit	Source
affp	880.40	kJ/mol	NIST Webbook
basg	848.60	kJ/mol	NIST Webbook
gf	10.32	kJ/mol	Joback Method
hf	-101.95	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	57.18	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.264		Crippen Method
mcvol	144.070	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
tb	602.04	K	Joback Method
tc	847.62	K	Joback Method
tf	356.90	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.03	J/mol×K	602.04	Joback Method
cpg	314.54	J/mol×K	642.97	Joback Method
cpg	325.26	J/mol×K	683.90	Joback Method
cpg	335.18	J/mol×K	724.83	Joback Method
cpg	344.35	J/mol×K	765.76	Joback Method
cpg	352.76	J/mol×K	806.69	Joback Method
cpg	360.44	J/mol×K	847.62	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=C32467666&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