3-CH3S-C6H4-COCH3

Inchi: InChI=1S/C9H10OS/c1-7(10)8-4-3-5-9(6-8)11-2/h3-6H,1-2H3
InchiKey: PJGDIRACIXOKQW-UHFFFAOYSA-N
Formula: C9H10OS
SMILES: CSc1cccc(C(C)=O)c1
Mol. weight [g/mol]: 166.24
CAS: 1441-99-2

Physical Properties

Property code	Value	Unit	Source
affp	866.60	kJ/mol	NIST Webbook
basg	834.70	kJ/mol	NIST Webbook
gf	31.88	kJ/mol	Joback Method
hf	-74.74	kJ/mol	Joback Method
hfus	18.45	kJ/mol	Joback Method
hvap	52.13	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.611		Crippen Method
mcvol	131.830	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
tb	559.63	K	Joback Method
tc	800.44	K	Joback Method
tf	314.46	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.71	J/mol×K	559.63	Joback Method
cpg	293.43	J/mol×K	599.76	Joback Method
cpg	305.31	J/mol×K	639.90	Joback Method
cpg	316.36	J/mol×K	680.03	Joback Method
cpg	326.60	J/mol×K	720.17	Joback Method
cpg	336.07	J/mol×K	760.30	Joback Method
cpg	344.78	J/mol×K	800.44	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=C1441992&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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