5-(Methylthio)-Salicylic acid, O,O'-dimethyl-

Inchi: InChI=1S/C10H12O3S/c1-12-9-5-4-7(14-3)6-8(9)10(11)13-2/h4-6H,1-3H3
InchiKey: ZKFYLVYMPYJXPS-UHFFFAOYSA-N
Formula: C10H12O3S
SMILES: COC(=O)c1cc(SC)ccc1OC
Mol. weight [g/mol]: 212.26

Physical Properties

Property code	Value	Unit	Source
gf	-179.33	kJ/mol	Joback Method
hf	-371.29	kJ/mol	Joback Method
hfus	23.02	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.204		Crippen Method
mcvol	157.660	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1751.00		NIST Webbook
tb	632.33	K	Joback Method
tc	862.46	K	Joback Method
tf	382.71	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.88	J/mol×K	632.33	Joback Method
cpg	385.85	J/mol×K	670.69	Joback Method
cpg	398.05	J/mol×K	709.04	Joback Method
cpg	409.46	J/mol×K	747.40	Joback Method
cpg	420.06	J/mol×K	785.75	Joback Method
cpg	429.81	J/mol×K	824.11	Joback Method
cpg	438.71	J/mol×K	862.46	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374801&Units=SI

Legend

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume