5-(Methylthio)salicylic acid, methyl ester

Inchi: InChI=1S/C9H10O3S/c1-12-9(11)7-5-6(13-2)3-4-8(7)10/h3-5,10H,1-2H3
InchiKey: IBKJRMIYOXLDIF-UHFFFAOYSA-N
Formula: C9H10O3S
SMILES: COC(=O)c1cc(SC)ccc1O
Mol. weight [g/mol]: 198.24

Physical Properties

Property code	Value	Unit	Source
gf	-227.74	kJ/mol	Joback Method
hf	-384.27	kJ/mol	Joback Method
hfus	25.42	kJ/mol	Joback Method
hvap	67.55	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.901		Crippen Method
mcvol	143.570	ml/mol	McGowan Method
pc	4140.93	kPa	Joback Method
rinpol	1613.00		NIST Webbook
rinpol	1613.00		NIST Webbook
tb	662.67	K	Joback Method
tc	908.85	K	Joback Method
tf	448.41	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.78	J/mol×K	662.67	Joback Method
cpg	358.70	J/mol×K	703.70	Joback Method
cpg	368.86	J/mol×K	744.73	Joback Method
cpg	378.32	J/mol×K	785.76	Joback Method
cpg	387.14	J/mol×K	826.79	Joback Method
cpg	395.38	J/mol×K	867.82	Joback Method
cpg	403.09	J/mol×K	908.85	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=U374459&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