Methyl 5-methoxysalicylate

Other names: 2-Hydroxy-5-methoxybenzoic acid methyl ester
Inchi: InChI=1S/C9H10O4/c1-12-6-3-4-8(10)7(5-6)9(11)13-2/h3-5,10H,1-2H3
InchiKey: DFNBGZODMHWKKK-UHFFFAOYSA-N
Formula: C9H10O4
SMILES: COC(=O)c1cc(OC)ccc1O
Mol. weight [g/mol]: 182.18

Physical Properties

Property code	Value	Unit	Source
hf	-612.17	kJ/mol	Cheméo Relay (1.0)
hfus	22.48	kJ/mol	Joback Method
ie	7.97	eV	Cheméo Relay (1.0)
log10ws	-2.49		Cheméo Relay (1.0)
logp	1.187		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
rinpol	1448.20		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1448.20		NIST Webbook
tb	551.28	K	Cheméo Relay (1.0)
tc	771.67	K	Cheméo Relay (1.0)
tf	327.55	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.39	J/mol×K	616.31	Joback Method
cpg	336.25	J/mol×K	653.92	Joback Method
cpg	346.47	J/mol×K	691.52	Joback Method
cpg	356.09	J/mol×K	729.13	Joback Method
cpg	365.12	J/mol×K	766.73	Joback Method
cpg	373.62	J/mol×K	804.34	Joback Method
cpg	381.62	J/mol×K	841.94	Joback Method
dvisc	0.0004335	Pa×s	436.24	Joback Method

dvisc	0.0002352	Pa×s	466.25	Joback Method
dvisc	0.0001374	Pa×s	496.26	Joback Method
dvisc	0.0000854	Pa×s	526.28	Joback Method
dvisc	0.0000558	Pa×s	556.29	Joback Method
dvisc	0.0000381	Pa×s	586.30	Joback Method
dvisc	0.0000270	Pa×s	616.31	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2905820&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
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