Methyl 4-methoxysalicylate

Other names:	Benzoic acid, 2-hydroxy-4-methoxy-, methyl ester
	Methyl 2-hydroxy-4-methoxybenzoate
Inchi:	InChI=1S/C9H10O4/c1-12-6-3-4-7(8(10)5-6)9(11)13-2/h3-5,10H,1-2H3
InchiKey:	ZICRWXFGZCVTBZ-UHFFFAOYSA-N
Formula:	C9H10O4
SMILES:	COC(=O)c1ccc(OC)cc1O
Mol. weight [g/mol]:	182.17
CAS:	5446-02-6

Physical Properties

Property code	Value	Unit	Source
gf	-365.86	kJ/mol	Joback Method
hf	-558.36	kJ/mol	Joback Method
hfus	22.48	kJ/mol	Joback Method
hvap	63.15	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.187		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
rinpol	1400.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1490.80		NIST Webbook
ripol	2217.00		NIST Webbook
ripol	2217.00		NIST Webbook
tb	616.31	K	Joback Method
tc	841.94	K	Joback Method
tf	436.24	K	Joback Method
vc	0.440	m3/kmol	Joback Method

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	526.27	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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5446026&Units=SI
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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume