methyl 3-methoxysalicylate

Other names: Methyl 2-hydroxy-3-methoxybenzoate
Inchi: InChI=1S/C9H10O4/c1-12-7-5-3-4-6(8(7)10)9(11)13-2/h3-5,10H,1-2H3
InchiKey: BWRCJLJJIXYLNV-UHFFFAOYSA-N
Formula: C9H10O4
SMILES: COC(=O)c1cccc(OC)c1O
Mol. weight [g/mol]: 182.17
CAS: 6342-70-7

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	1417.00		NIST Webbook
rinpol	1459.50		NIST Webbook
ripol	2239.00		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

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=C6342707&Units=SI

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

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