Benzoic acid, 2-hydroxy-6-methyl-, methyl ester

Other names: 2,6-Cresotic acid, methyl ester
Methyl 6-methylsalicylate

Inchi: InChI=1S/C9H10O3/c1-6-4-3-5-7(10)8(6)9(11)12-2/h3-5,10H,1-2H3

InchiKey: GPNCYIZKJTXKRO-UHFFFAOYSA-N

Formula: C9H10O3

SMILES: COC(=O)c1c(C)cccc1O

Mol. weight [g/mol]: 166.17

CAS: 33528-09-5

Physical Properties

Property code	Value	Unit	Source
gf	-260.86	kJ/mol	Joback Method
hf	-426.14	kJ/mol	Joback Method
hfus	21.29	kJ/mol	Joback Method
hvap	60.74	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.487		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
ripol	1970.00		NIST Webbook
tb	593.89	K	Joback Method
tc	822.63	K	Joback Method
tf	414.01	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.95	J/mol×K	593.89	Joback Method
cpg	313.95	J/mol×K	632.01	Joback Method
cpg	324.24	J/mol×K	670.14	Joback Method
cpg	333.88	J/mol×K	708.26	Joback Method
cpg	342.92	J/mol×K	746.38	Joback Method
cpg	351.43	J/mol×K	784.51	Joback Method

cpg	359.45	J/mol×K	822.63	Joback Method
dvisc	0.0007214	Pa×s	414.01	Joback Method
dvisc	0.0003744	Pa×s	443.99	Joback Method
dvisc	0.0002111	Pa×s	473.97	Joback Method
dvisc	0.0001274	Pa×s	503.95	Joback Method
dvisc	0.0000814	Pa×s	533.93	Joback Method
dvisc	0.0000546	Pa×s	563.91	Joback Method
dvisc	0.0000381	Pa×s	593.89	Joback Method

Sources

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=C33528095&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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