Benzoic acid, 3-formyl-2,4-dihydroxy-6-methyl-, methyl ester

Othernames: Methyl haematommate
Methyl hematommate
Inchi: InChI=1S/C10H10O5/c1-5-3-7(12)6(4-11)9(13)8(5)10(14)15-2/h3-4,12-13H,1-2H3
InchiKey: PXFMUVDLJWXOQM-UHFFFAOYSA-N
Formula: C10H10O5
SMILES: COC(=O)c1c(C)cc(O)c(C=O)c1O
Mol. weight [g/mol]: 210.18
CAS: 34874-90-3

Physical Properties

Property code	Value	Unit	Source
gf	-516.21	kJ/mol	Joback Method
hf	-721.14	kJ/mol	Joback Method
hfus	31.56	kJ/mol	Joback Method
hvap	83.36	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.005		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
pc	4697.74	kPa	Joback Method
rinpol	1669.00		NIST Webbook
rinpol	1669.00		NIST Webbook
tb	751.03	K	Joback Method
tc	985.48	K	Joback Method
tf	591.52	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.94	J/mol×K	751.03	Joback Method
cpg	442.47	J/mol×K	946.40	Joback Method
cpg	434.30	J/mol×K	907.33	Joback Method
cpg	426.06	J/mol×K	868.25	Joback Method
cpg	417.65	J/mol×K	829.18	Joback Method

cpg	408.98	J/mol×K	790.10	Joback Method
cpg	450.69	J/mol×K	985.48	Joback Method
dvisc	0.0000014	Pa×s	751.03	Joback Method
dvisc	0.0000019	Pa×s	724.44	Joback Method
dvisc	0.0000027	Pa×s	697.86	Joback Method
dvisc	0.0000040	Pa×s	671.27	Joback Method
dvisc	0.0000061	Pa×s	644.69	Joback Method
dvisc	0.0000095	Pa×s	618.11	Joback Method
dvisc	0.0000156	Pa×s	591.52	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=C34874903&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume