

meth yl gallate

Inchi: InChI=1S/C8H8O5/c1-13-8(12)4-2-5(9)7(11)6(10)3-4/h2-3,9-11H,1H3
InchiKey: FBSFWRHWHYMIQG-UHFFFAOYSA-N
Formula: C8H8O5
SMILES: COC(=O)c1cc(O)c(O)c(O)c1
Mol. weight [g/mol]: 184.15

Physical Properties

Property code	Value	Unit	Source
gf	-568.89	kJ/mol	Joback Method
hf	-748.65	kJ/mol	Joback Method
hfus	30.65	kJ/mol	Joback Method
hvap	83.88	kJ/mol	Joback Method
log10ws	-1.24		Estimated Solubility Method
log10ws	-1.24		Aqueous Solubility Prediction Method
logp	0.590		Crippen Method
mcvol	124.870	ml/mol	McGowan Method
pc	7406.07	kPa	Joback Method
tb	727.27	K	Joback Method
tc	976.22	K	Joback Method
tf	504.40	K	Aqueous Solubility Prediction Method
vc	0.297	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.79	J/mol×K	727.27	Joback Method
cpg	343.51	J/mol×K	768.76	Joback Method
cpg	351.03	J/mol×K	810.25	Joback Method
cpg	358.55	J/mol×K	851.75	Joback Method
cpg	366.26	J/mol×K	893.24	Joback Method
cpg	374.35	J/mol×K	934.73	Joback Method
cpg	383.02	J/mol×K	976.22	Joback Method

dvisc	0.0000014	Pa×s	613.66	Joback Method
dvisc	0.0000009	Pa×s	632.60	Joback Method
dvisc	0.0000006	Pa×s	651.53	Joback Method
dvisc	0.0000004	Pa×s	670.46	Joback Method
dvisc	0.0000003	Pa×s	689.40	Joback Method
dvisc	0.0000002	Pa×s	708.34	Joback Method
dvisc	0.0000001	Pa×s	727.27	Joback Method

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

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

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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