Benzoic acid, 3,4,5-trimethoxy-

Other names:	Eudesmic acid
	Gallic acid trimethyl ether
	Tri-O-methylgallic acid
	Veratric acid, 5-methoxy-
	3,4,5-Trimethoxybenzoic acid
	Trimethylgallic acid
	NSC 2525
Inchi:	InChI=1S/C10H12O5/c1-13-7-4-6(10(11)12)5-8(14-2)9(7)15-3/h4-5H,1-3H3,(H,11,12)
InchiKey:	SJSOFNCYXJUNBT-UHFFFAOYSA-N
Formula:	C10H12O5
SMILES:	COc1cc(C(=O)O)cc(OC)c1OC
Mol. weight [g/mol]:	212.20
CAS:	118-41-2

Physical Properties

Property code	Value	Unit	Source
gf	-463.90	kJ/mol	Joback Method
hf	-709.08	kJ/mol	Joback Method
hfus	23.78	kJ/mol	Joback Method
hsub	131.20 ± 0.80	kJ/mol	NIST Webbook
hvap	72.77	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.411		Crippen Method
mcvol	153.050	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
rinpol	1771.80		NIST Webbook
rinpol	1771.80		NIST Webbook
tb	683.13	K	Joback Method
tc	881.29	K	Joback Method
tf	443.88	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.01	J/mol×K	848.26	Joback Method
cpg	449.51	J/mol×K	881.29	Joback Method
cpg	395.28	J/mol×K	683.13	Joback Method
cpg	405.78	J/mol×K	716.16	Joback Method
cpg	415.73	J/mol×K	749.18	Joback Method
cpg	425.10	J/mol×K	782.21	Joback Method
cpg	433.87	J/mol×K	815.24	Joback Method
dvisc	0.0000353	Pa×s	683.13	Joback Method
dvisc	0.0000483	Pa×s	643.25	Joback Method
dvisc	0.0005426	Pa×s	443.88	Joback Method
dvisc	0.0002852	Pa×s	483.75	Joback Method
dvisc	0.0001653	Pa×s	523.63	Joback Method
dvisc	0.0001035	Pa×s	563.50	Joback Method
dvisc	0.0000690	Pa×s	603.38	Joback Method
hfust	29.90	kJ/mol	444.50	NIST Webbook
hsubt	127.90 ± 0.80	kJ/mol	363.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	499.20	K	1.30	NIST Webbook

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=C118412&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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume