

Benzoic acid, 3,4-dimethoxy-, methyl ester

Other names:	Veratric acid, methyl ester Methyl veratrate Methyl 3,4-dimethoxybenzoate 3,4-Dimethoxybenzoic acid methyl ester Methyl ester of 3,4-Dimethoxybenzoic acid
Inchi:	InChI=1S/C10H12O4/c1-12-8-5-4-7(10(11)14-3)6-9(8)13-2/h4-6H,1-3H3
InchiKey:	BIGQPYZPEWAPBG-UHFFFAOYSA-N
Formula:	C10H12O4
SMILES:	COC(=O)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]:	196.20
CAS:	2150-38-1

Physical Properties

Property code	Value	Unit	Source
gf	-317.45	kJ/mol	Joback Method
hf	-545.38	kJ/mol	Joback Method
hfus	20.08	kJ/mol	Joback Method
hvap	55.43	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.490		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	1520.00		NIST Webbook
rinpol	1599.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1543.00		NIST Webbook
rinpol	1599.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1548.00		NIST Webbook
tb	573.20	K	NIST Webbook
tb	556.20	K	NIST Webbook
tc	796.18	K	Joback Method
tf	370.54	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.19	J/mol×K	585.97	Joback Method
cpg	359.83	J/mol×K	621.00	Joback Method
cpg	371.90	J/mol×K	656.04	Joback Method
cpg	383.37	J/mol×K	691.07	Joback Method
cpg	394.23	J/mol×K	726.11	Joback Method
cpg	404.44	J/mol×K	761.14	Joback Method
cpg	413.99	J/mol×K	796.18	Joback Method
dvisc	0.0008149	Pa×s	370.54	Joback Method
dvisc	0.0005311	Pa×s	406.45	Joback Method
dvisc	0.0003711	Pa×s	442.35	Joback Method
dvisc	0.0002736	Pa×s	478.25	Joback Method
dvisc	0.0002105	Pa×s	514.16	Joback Method
dvisc	0.0001676	Pa×s	550.07	Joback Method
dvisc	0.0001372	Pa×s	585.97	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	403.70	K	0.30	NIST Webbook

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=C2150381&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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