2,4,6-TRIMETHOXYBENZALDEHYDE

Other names: Benzaldehyde, 2,4,6-trimethoxy-
Inchi: InChI=1S/C10H12O4/c1-12-7-4-9(13-2)8(6-11)10(5-7)14-3/h4-6H,1-3H3
InchiKey: CRBZVDLXAIFERF-UHFFFAOYSA-N
Formula: C10H12O4
SMILES: COc1cc(OC)c(C=O)c(OC)c1
Mol. weight [g/mol]: 196.20

Physical Properties

Property code	Value	Unit	Source
hf	-516.00	kJ/mol	Cheméo Relay (1.0)
hfus	20.38	kJ/mol	Joback Method
hvap	75.57	kJ/mol	Cheméo Relay (1.0)
ie	8.22	eV	Cheméo Relay (1.0)
log10ws	-2.51		Cheméo Relay (1.0)
logp	1.525		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
tb	577.08	K	Cheméo Relay (1.0)
tf	355.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.43	J/mol×K	585.74	Joback Method
cpg	359.52	J/mol×K	620.16	Joback Method
cpg	371.11	J/mol×K	654.57	Joback Method
cpg	382.17	J/mol×K	688.99	Joback Method
cpg	392.68	J/mol×K	723.40	Joback Method
cpg	402.61	J/mol×K	757.82	Joback Method
cpg	411.94	J/mol×K	792.23	Joback Method
dvisc	0.0007464	Pa×s	375.13	Joback Method
dvisc	0.0005076	Pa×s	410.23	Joback Method
dvisc	0.0003668	Pa×s	445.33	Joback Method
dvisc	0.0002780	Pa×s	480.44	Joback Method
dvisc	0.0002187	Pa×s	515.54	Joback Method

dvisc	0.0001775	Pa×s	550.64	Joback Method
dvisc	0.0001477	Pa×s	585.74	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C830795&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point