Propan-1-one, 1-(3,4-dimethoxyphenyl)-

Other names:	Propioveratrone
	1-(3,4-Dimethoxyphenyl)-1-propanone
	1-Propanone, 1-(3,4-dimethoxyphenyl)-
	3,4-Dimethoxyphenyl ethyl ketone
	3,4-Dimethoxypropiophenone
	3',4'-Dimethoxypropiophenone
	Propan-1-one, 1-(3,4-dimethoxyphenyl)-
Inchi:	InChI=1S/C11H14O3/c1-4-9(12)8-5-6-10(13-2)11(7-8)14-3/h5-7H,4H2,1-3H3
InchiKey:	SBMSBQOMJGZBRY-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	CCC(=O)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]:	194.23

Physical Properties

Property code	Value	Unit	Source
hfus	21.48	kJ/mol	Joback Method
ie	8.29	eV	Cheméo Relay (1.0)
log10ws	-2.55		Cheméo Relay (1.0)
logp	2.296		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
tb	563.40	K	Cheméo Relay (1.0)
tf	363.42	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.29	J/mol×K	586.43	Joback Method
cpg	383.95	J/mol×K	621.28	Joback Method
cpg	396.95	J/mol×K	656.13	Joback Method
cpg	409.28	J/mol×K	690.97	Joback Method
cpg	420.93	J/mol×K	725.82	Joback Method
cpg	431.89	J/mol×K	760.67	Joback Method

cpg	442.17	J/mol×K	795.52	Joback Method
dvisc	0.0010431	Pa×s	359.58	Joback Method
dvisc	0.0006535	Pa×s	397.39	Joback Method
dvisc	0.0004440	Pa×s	435.20	Joback Method
dvisc	0.0003209	Pa×s	473.01	Joback Method
dvisc	0.0002434	Pa×s	510.81	Joback Method
dvisc	0.0001918	Pa×s	548.62	Joback Method
dvisc	0.0001558	Pa×s	586.43	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=C1835047&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
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point