3,4-Dimethoxyphenylacetone

Other names:	Veratryl acetone
	2-Propanone, 1-(3,4-dimethoxyphenyl)-
	3,4-Dimethoxybenzyl methyl ketone
	1-(3,4-Dimethoxyphenyl)-2-propanone
	Veratryl-2-propanone
	1-(3,4-dimethoxyphenyl)acetone
Inchi:	InChI=1S/C11H14O3/c1-8(12)6-9-4-5-10(13-2)11(7-9)14-3/h4-5,7H,6H2,1-3H3
InchiKey:	UMYZWICEDUEWIM-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	COc1ccc(CC(C)=O)cc1OC
Mol. weight [g/mol]:	194.23
CAS:	776-99-8

Physical Properties

Property code	Value	Unit	Source
gf	-204.03	kJ/mol	Joback Method
hf	-433.80	kJ/mol	Joback Method
hfus	21.48	kJ/mol	Joback Method
hvap	55.25	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	1.835		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
ripol	2470.00		NIST Webbook
tb	586.43	K	Joback Method
tc	795.52	K	Joback Method
tf	359.58	K	Joback Method
vc	0.586	m3/kmol	Joback Method

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	473.00	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

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=C776998&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume