

1-Propanone, 1-(2,4-dimethoxyphenyl)-

Other names:	Propiophenone, 2',4'-dimethoxy- 2',4'-Dimethoxypropiophenone Propan-1-one, 1-(2,4-dimethoxyphenyl)-
Inchi:	InChI=1S/C11H14O3/c1-4-10(12)9-6-5-8(13-2)7-11(9)14-3/h5-7H,4H2,1-3H3
InchiKey:	MIAQBCIDZSELDU-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	CCC(=O)c1ccc(OC)cc1OC
Mol. weight [g/mol]:	194.23
CAS:	831-00-5

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	-2.79		Crippen Method
logp	2.296		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
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/molxK	586.43	Joback Method
cpg	383.95	J/molxK	621.28	Joback Method
cpg	396.95	J/molxK	656.13	Joback Method
cpg	409.28	J/molxK	690.97	Joback Method
cpg	420.93	J/molxK	725.82	Joback Method
cpg	431.89	J/molxK	760.67	Joback Method

cpg	442.17	J/mol×K	795.52	Joback Method
dvisc	0.0010431	Paxs	359.58	Joback Method
dvisc	0.0006535	Paxs	397.39	Joback Method
dvisc	0.0004440	Paxs	435.20	Joback Method
dvisc	0.0003209	Paxs	473.00	Joback Method
dvisc	0.0002434	Paxs	510.81	Joback Method
dvisc	0.0001918	Paxs	548.62	Joback Method
dvisc	0.0001558	Paxs	586.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C831005&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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