

2',4'-Dimethoxyacetophenone

Other names:	2,4-Dimethoxyacetophenone Ethanone, 1-(2,4-dimethoxyphenyl)- Acetophenone, 2',4'-dimethoxy- 1-(2,4-Dimethoxy-phenyl)-ethanone Resacetophenone dimethyl ether 2',4'-Dihydroxyacetophenone, dimethyl ether 1-(2,4-dimethoxyphenyl)ethan-1-one
Inchi:	InChI=1S/C10H12O3/c1-7(11)9-5-4-8(12-2)6-10(9)13-3/h4-6H,1-3H3
InchiKey:	VQTDPCRSXHFMOL-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	COc1ccc(C(C)=O)c(OC)c1
Mol. weight [g/mol]:	180.20
CAS:	829-20-9

Physical Properties

Property code	Value	Unit	Source
gf	-212.45	kJ/mol	Joback Method
hf	-413.16	kJ/mol	Joback Method
hfus	18.89	kJ/mol	Joback Method
hvap	53.02	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.906		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	1586.30		NIST Webbook
rinpol	1586.30		NIST Webbook
rinpol	1593.00		NIST Webbook
tb	561.20	K	NIST Webbook
tc	776.08	K	Joback Method
tf	348.31	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.48	J/mol×K	563.55	Joback Method
cpg	336.25	J/mol×K	598.97	Joback Method
cpg	348.42	J/mol×K	634.39	Joback Method
cpg	359.98	J/mol×K	669.82	Joback Method
cpg	370.92	J/mol×K	705.24	Joback Method
cpg	381.23	J/mol×K	740.66	Joback Method
cpg	390.91	J/mol×K	776.08	Joback Method
dvisc	0.0010565	Paxs	348.31	Joback Method
dvisc	0.0006746	Paxs	384.18	Joback Method
dvisc	0.0004650	Paxs	420.06	Joback Method
dvisc	0.0003399	Paxs	455.93	Joback Method
dvisc	0.0002601	Paxs	491.80	Joback Method
dvisc	0.0002064	Paxs	527.68	Joback Method
dvisc	0.0001686	Paxs	563.55	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C829209&Units=SI

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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

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