

Ethanone, 1-(3,4,5-trimethoxyphenyl)-

Other names:	3',4',5'-Trimethoxyacetophenone 3,4,5-Trimethoxyacetophenone Acetophenone, 3',4',5'-trimethoxy
Inchi:	InChI=1S/C11H14O4/c1-7(12)8-5-9(13-2)11(15-4)10(6-8)14-3/h5-6H,1-4H3
InchiKey:	VUGQIIQFXXZJU-UHFFFAOYSA-N
Formula:	C11H14O4
SMILES:	COc1cc(C(C)=O)cc(OC)c1OC
Mol. weight [g/mol]:	210.23
CAS:	1136-86-3

Physical Properties

Property code	Value	Unit	Source
gf	-318.66	kJ/mol	Joback Method
hf	-577.49	kJ/mol	Joback Method
hfus	22.28	kJ/mol	Joback Method
hvap	58.32	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.915		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1632.00		NIST Webbook
rinpol	1632.00		NIST Webbook
tb	613.83	K	Joback Method
tc	821.66	K	Joback Method
tf	394.33	K	Joback Method
vc	0.604	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.23	J/molxK	613.83	Joback Method
cpg	407.53	J/molxK	648.47	Joback Method
cpg	420.23	J/molxK	683.11	Joback Method
cpg	432.28	J/molxK	717.75	Joback Method

cpg	443.68	J/molxK	752.39	Joback Method
cpg	454.40	J/molxK	787.02	Joback Method
cpg	464.40	J/molxK	821.66	Joback Method
dvisc	0.0006543	Paxs	394.33	Joback Method
dvisc	0.0004404	Paxs	430.91	Joback Method
dvisc	0.0003154	Paxs	467.50	Joback Method
dvisc	0.0002371	Paxs	504.08	Joback Method
dvisc	0.0001853	Paxs	540.66	Joback Method
dvisc	0.0001494	Paxs	577.25	Joback Method
dvisc	0.0001235	Paxs	613.83	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	446.70	K	1.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1136863&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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