1-(2,4,5-Trimethoxyphenyl)propan-2-one

Inchi: InChI=1S/C12H16O4/c1-8(13)5-9-6-11(15-3)12(16-4)7-10(9)14-2/h6-7H,5H2,1-4H3
InchiKey: AQZHZTTUVYQMIN-UHFFFAOYSA-N
Formula: C12H16O4
SMILES: COc1cc(OC)c(OC)cc1CC(C)=O
Mol. weight [g/mol]: 224.25
CAS: 2020-90-8

Physical Properties

Property code	Value	Unit	Source
gf	-310.24	kJ/mol	Joback Method
hf	-598.13	kJ/mol	Joback Method
hfus	24.87	kJ/mol	Joback Method
hvap	60.54	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	1.844		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	1751.10		NIST Webbook
rinpol	1751.10		NIST Webbook
tb	636.71	K	Joback Method
tc	841.45	K	Joback Method
tf	405.60	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.68	J/mol×K	636.71	Joback Method
cpg	457.73	J/mol×K	670.83	Joback Method
cpg	471.10	J/mol×K	704.96	Joback Method
cpg	483.78	J/mol×K	739.08	Joback Method
cpg	495.73	J/mol×K	773.20	Joback Method
cpg	506.94	J/mol×K	807.33	Joback Method
cpg	517.39	J/mol×K	841.45	Joback Method

dvisc	0.0006338	Pa×s	405.60	Joback Method
dvisc	0.0004193	Pa×s	444.12	Joback Method
dvisc	0.0002963	Pa×s	482.64	Joback Method
dvisc	0.0002204	Pa×s	521.15	Joback Method
dvisc	0.0001707	Pa×s	559.67	Joback Method
dvisc	0.0001367	Pa×s	598.19	Joback Method
dvisc	0.0001124	Pa×s	636.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2020908&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume