

Isopropyl 3,4,5-trimethoxyphenyl ketone

Inchi:	InChI=1S/C13H18O4/c1-8(2)12(14)9-6-10(15-3)13(17-5)11(7-9)16-4/h6-8H,1-5H3
InchiKey:	WCOTWXLJGZKQQE-UHFFFAOYSA-N
Formula:	C13H18O4
SMILES:	COc1cc(C(=O)C(C)C)cc(OC)c1OC
Mol. weight [g/mol]:	238.28

Physical Properties

Property code	Value	Unit	Source
gf	-304.26	kJ/mol	Joback Method
hf	-624.05	kJ/mol	Joback Method
hfus	23.94	kJ/mol	Joback Method
hvap	62.38	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.551		Crippen Method
mvol	189.450	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	1790.00		NIST Webbook
rinpol	1790.00		NIST Webbook
tb	659.15	K	Joback Method
tc	864.76	K	Joback Method
tf	401.87	K	Joback Method
vc	0.710	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.17	J/molxK	659.15	Joback Method
cpg	510.15	J/molxK	693.42	Joback Method
cpg	524.36	J/molxK	727.69	Joback Method
cpg	537.78	J/molxK	761.95	Joback Method
cpg	550.38	J/molxK	796.22	Joback Method
cpg	562.14	J/molxK	830.49	Joback Method
cpg	573.06	J/molxK	864.76	Joback Method
dvisc	0.0007007	Paxs	401.87	Joback Method

dvisc	0.0004270	Paxs	444.75	Joback Method
dvisc	0.0002839	Paxs	487.63	Joback Method
dvisc	0.0002016	Paxs	530.51	Joback Method
dvisc	0.0001507	Paxs	573.39	Joback Method
dvisc	0.0001173	Paxs	616.27	Joback Method
dvisc	0.0000943	Paxs	659.15	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=R204243&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
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

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