

Methyl 3,4,6-trimethoxy-2-methyl-benzoate

Inchi:	InChI=1S/C12H16O5/c1-7-10(12(13)17-5)8(14-2)6-9(15-3)11(7)16-4/h6H,1-5H3
InchiKey:	JVDDGFUMQFNKGJ-UHFFFAOYSA-N
Formula:	C12H16O5
SMILES:	<chem>COC(=O)c1c(OC)cc(OC)c(OC)c1C</chem>
Mol. weight [g/mol]:	240.25

Physical Properties

Property code	Value	Unit	Source
gf	-424.87	kJ/mol	Joback Method
hf	-741.82	kJ/mol	Joback Method
hfus	25.67	kJ/mol	Joback Method
hvap	63.62	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	1.807		Crippen Method
mcvol	181.230	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	1706.00		NIST Webbook
rinpol	1706.00		NIST Webbook
tb	664.11	K	Joback Method
tc	867.85	K	Joback Method
tf	440.35	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.52	J/molxK	664.11	Joback Method
cpg	530.23	J/molxK	833.90	Joback Method
cpg	519.37	J/molxK	799.94	Joback Method
cpg	507.73	J/molxK	765.98	Joback Method
cpg	495.35	J/molxK	732.02	Joback Method
cpg	482.27	J/molxK	698.07	Joback Method
cpg	540.27	J/molxK	867.85	Joback Method
dvisc	0.0000883	Paxs	664.11	Joback Method

dvisc	0.0001057	Paxs	626.82	Joback Method
dvisc	0.0001293	Paxs	589.52	Joback Method
dvisc	0.0001627	Paxs	552.23	Joback Method
dvisc	0.0002116	Paxs	514.94	Joback Method
dvisc	0.0002867	Paxs	477.64	Joback Method
dvisc	0.0004089	Paxs	440.35	Joback Method

Sources

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=R273888&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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