Benzoic acid, 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C15H14O4/c1-17-12-9-6-10-13(18-2)14(12)19-15(16)11-7-4-3-5-8-11/h3-10H,1
InchiKey: SVMPWMYCQQADHO-UHFFFAOYSA-N
Formula: C15H14O4
SMILES: COc1cccc(OC)c1OC(=O)c1ccccc1
Mol. weight [g/mol]: 258.27

Physical Properties

Property code	Value	Unit	Source
gf	-162.94	kJ/mol	Joback Method
hf	-412.05	kJ/mol	Joback Method
hfus	27.07	kJ/mol	Joback Method
hvap	68.84	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	2.923		Crippen Method
mcvol	193.870	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	2096.00		NIST Webbook
rinpol	2096.00		NIST Webbook
tb	727.05	K	Joback Method
tc	959.54	K	Joback Method
tf	453.31	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.43	J/mol×K	727.05	Joback Method
cpg	577.76	J/mol×K	920.79	Joback Method
cpg	567.78	J/mol×K	882.04	Joback Method
cpg	556.66	J/mol×K	843.29	Joback Method
cpg	544.39	J/mol×K	804.55	Joback Method
cpg	530.98	J/mol×K	765.80	Joback Method
cpg	586.59	J/mol×K	959.54	Joback Method
dvisc	0.0000828	Pa×s	727.05	Joback Method

dvisc	0.0001023	Pa×s	681.43	Joback Method
dvisc	0.0001304	Pa×s	635.80	Joback Method
dvisc	0.0001724	Pa×s	590.18	Joback Method
dvisc	0.0002390	Pa×s	544.56	Joback Method
dvisc	0.0003516	Pa×s	498.93	Joback Method
dvisc	0.0005592	Pa×s	453.31	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=U368912&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