3,4-Dimethoxybenzoic anhydride

Inchi: InChI=1S/C18H18O7/c1-21-13-7-5-11(9-15(13)23-3)17(19)25-18(20)12-6-8-14(22-2)16(1
InchiKey: PJZFUQAHDYSNLZ-UHFFFAOYSA-N
Formula: C18H18O7
SMILES: COc1ccc(C(=O)OC(=O)c2ccc(OC)c(OC)c2)cc1OC
Mol. weight [g/mol]: 346.33

Physical Properties

Property code	Value	Unit	Source
gf	-495.86	kJ/mol	Joback Method
hf	-873.93	kJ/mol	Joback Method
hfus	38.04	kJ/mol	Joback Method
hvap	88.40	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	2.718		Crippen Method
mcvol	249.450	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	2932.70		NIST Webbook
rinpol	2932.70		NIST Webbook
tb	904.36	K	Joback Method
tc	1130.99	K	Joback Method
tf	606.55	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.29	J/mol×K	904.36	Joback Method
cpg	754.76	J/mol×K	942.13	Joback Method
cpg	764.67	J/mol×K	979.90	Joback Method
cpg	772.97	J/mol×K	1017.67	Joback Method
cpg	779.63	J/mol×K	1055.45	Joback Method
cpg	784.60	J/mol×K	1093.22	Joback Method
cpg	787.82	J/mol×K	1130.99	Joback Method
dvisc	0.0001659	Pa×s	606.55	Joback Method

dvisc	0.0001145	Pa×s	656.18	Joback Method
dvisc	0.0000833	Pa×s	705.82	Joback Method
dvisc	0.0000632	Pa×s	755.45	Joback Method
dvisc	0.0000496	Pa×s	805.09	Joback Method
dvisc	0.0000400	Pa×s	854.72	Joback Method
dvisc	0.0000331	Pa×s	904.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333905&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