(E)-1-(2-Hydroxy-4,6-dimethoxyphenyl)-3-(4-metho

Inchi: InChI=1S/C18H18O5/c1-21-13-7-4-12(5-8-13)6-9-15(19)18-16(20)10-14(22-2)11-17(18)2
InchiKey: CGIBCVBDFUTMPT-RMKNXTFCSA-N
Formula: C18H18O5
SMILES: COc1ccc(C=CC(=O)c2c(O)cc(OC)cc2OC)cc1
Mol. weight [g/mol]: 314.33
CAS: 64680-84-8

Physical Properties

Property code	Value	Unit	Source
gf	-221.71	kJ/mol	Joback Method
hf	-545.53	kJ/mol	Joback Method
hfus	40.44	kJ/mol	Joback Method
hvap	89.15	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.314		Crippen Method
mcvol	237.710	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	2964.90		NIST Webbook
rinpol	2964.90		NIST Webbook
tb	885.45	K	Joback Method
tc	1122.36	K	Joback Method
tf	606.28	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.18	J/mol×K	885.45	Joback Method
cpg	715.41	J/mol×K	924.94	Joback Method
cpg	727.75	J/mol×K	964.42	Joback Method
cpg	739.25	J/mol×K	1003.91	Joback Method
cpg	750.00	J/mol×K	1043.39	Joback Method
cpg	760.05	J/mol×K	1082.88	Joback Method
cpg	769.48	J/mol×K	1122.36	Joback Method

dvisc	0.0000312	Pa×s	606.28	Joback Method
dvisc	0.0000173	Pa×s	652.81	Joback Method
dvisc	0.0000104	Pa×s	699.34	Joback Method
dvisc	0.0000066	Pa×s	745.87	Joback Method
dvisc	0.0000045	Pa×s	792.39	Joback Method
dvisc	0.0000031	Pa×s	838.92	Joback Method
dvisc	0.0000023	Pa×s	885.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64680848&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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