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

Inchi: InChI=1S/C17H16O4/c1-20-13-10-15(19)17(16(11-13)21-2)14(18)9-8-12-6-4-3-5-7-12/h3
InchiKey: QKQLSQLKXBHUSO-CMDGGOBGSA-N
Formula: C17H16O4
SMILES: COc1cc(O)c(C(=O)C=Cc2ccccc2)c(OC)c1
Mol. weight [g/mol]: 284.31
CAS: 1775-97-9

Physical Properties

Property code	Value	Unit	Source
gf	-115.50	kJ/mol	Joback Method
hf	-381.20	kJ/mol	Joback Method
hfus	37.05	kJ/mol	Joback Method
hvap	83.85	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.305		Crippen Method
mcvol	217.750	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	2636.10		NIST Webbook
rinpol	2636.10		NIST Webbook
tb	835.17	K	Joback Method
tc	1077.37	K	Joback Method
tf	560.26	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.41	J/mol×K	835.17	Joback Method
cpg	634.78	J/mol×K	875.54	Joback Method
cpg	647.31	J/mol×K	915.90	Joback Method
cpg	659.08	J/mol×K	956.27	Joback Method
cpg	670.20	J/mol×K	996.64	Joback Method
cpg	680.77	J/mol×K	1037.01	Joback Method
cpg	690.89	J/mol×K	1077.37	Joback Method

dvisc	0.0000678	Pa×s	560.26	Joback Method
dvisc	0.0000352	Pa×s	606.08	Joback Method
dvisc	0.0000201	Pa×s	651.90	Joback Method
dvisc	0.0000123	Pa×s	697.72	Joback Method
dvisc	0.0000080	Pa×s	743.53	Joback Method
dvisc	0.0000055	Pa×s	789.35	Joback Method
dvisc	0.0000039	Pa×s	835.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1775979&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

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