Fumaric acid, monoamide, N-methyl-N-phenyl-, 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C19H19NO5/c1-20(14-8-5-4-6-9-14)17(21)12-13-18(22)25-19-15(23-2)10-7-11
InchiKey: OJUOGKFRRFMYMP-OUKQBFOZSA-N
Formula: C19H19NO5
SMILES: COc1cccc(OC)c1OC(=O)C=CC(=O)N(C)c1ccccc1
Mol. weight [g/mol]: 341.36

Physical Properties

Property code	Value	Unit	Source
gf	-67.18	kJ/mol	Joback Method
hf	-422.44	kJ/mol	Joback Method
hfus	42.25	kJ/mol	Joback Method
hvap	86.49	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.828		Crippen Method
mcvol	257.480	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	2879.00		NIST Webbook
tb	889.04	K	Joback Method
tc	1118.55	K	Joback Method
tf	575.71	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.66	J/mol×K	889.04	Joback Method
cpg	776.49	J/mol×K	927.29	Joback Method
cpg	788.05	J/mol×K	965.54	Joback Method
cpg	798.38	J/mol×K	1003.80	Joback Method
cpg	807.52	J/mol×K	1042.05	Joback Method
cpg	815.50	J/mol×K	1080.30	Joback Method
cpg	822.37	J/mol×K	1118.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357460&Units=SI

Legend

cpg:	Ideal gas heat capacity
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