Fumaric acid, monoamide, N,N-dimethyl-, 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C14H17NO5/c1-15(2)12(16)8-9-13(17)20-14-10(18-3)6-5-7-11(14)19-4/h5-9H,

InchiKey: HDHYZJNRYSPJCX-CMDGGOBGSA-N

Formula: C14H17NO5

SMILES: COc1cccc(OC)c1OC(=O)C=CC(=O)N(C)C

Mol. weight [g/mol]: 279.29

Physical Properties

Property code	Value	Unit	Source
gf	-221.69	kJ/mol	Joback Method
hf	-555.77	kJ/mol	Joback Method
hfus	35.26	kJ/mol	Joback Method
hvap	73.08	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.254		Crippen Method
mcvol	210.790	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	2432.00		NIST Webbook
tb	747.96	K	Joback Method
tc	957.82	K	Joback Method
tf	492.94	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.93	J/mol×K	747.96	Joback Method
cpg	594.48	J/mol×K	782.94	Joback Method
cpg	607.09	J/mol×K	817.91	Joback Method
cpg	618.78	J/mol×K	852.89	Joback Method
cpg	629.55	J/mol×K	887.87	Joback Method
cpg	639.41	J/mol×K	922.85	Joback Method
cpg	648.36	J/mol×K	957.82	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=U357457&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