Fumaric acid, monoamide, N-(2,4-dimethoxyphenyl)-, isopropyl ester

Inchi: InChI=1S/C15H19NO5/c1-10(2)21-15(18)8-7-14(17)16-12-6-5-11(19-3)9-13(12)20-4/h5-1

InchiKey: KFNWBZQRZYKFHT-BQYQJAHWSA-N

Formula: C15H19NO5

SMILES: COc1ccc(NC(=O)C=CC(=O)OC(C)C)c(OC)c1

Mol. weight [g/mol]: 293.32

Physical Properties

Property code	Value	Unit	Source
gf	-237.10	kJ/mol	Joback Method
hf	-595.75	kJ/mol	Joback Method
hfus	36.41	kJ/mol	Joback Method
hvap	79.31	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.150		Crippen Method
mcvol	224.880	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	2541.00		NIST Webbook
tb	808.13	K	Joback Method
tc	1021.60	K	Joback Method
tf	509.40	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.54	J/mol×K	808.13	Joback Method
cpg	662.82	J/mol×K	843.71	Joback Method
cpg	675.07	J/mol×K	879.29	Joback Method
cpg	686.29	J/mol×K	914.86	Joback Method
cpg	696.48	J/mol×K	950.44	Joback Method
cpg	705.65	J/mol×K	986.02	Joback Method
cpg	713.80	J/mol×K	1021.60	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=U357527&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