Fumaric acid, monoamide, N-(3,4-dimethoxyphenethyl)-, isopropyl ester

Inchi: InChI=1S/C17H23NO5/c1-12(2)23-17(20)8-7-16(19)18-10-9-13-5-6-14(21-3)15(11-13)22
InchiKey: PNPOZMCWMIKFFE-BQYQJAHWSA-N
Formula: C17H23NO5
SMILES: COc1ccc(CCNC(=O)C=CC(=O)OC(C)C)cc1OC
Mol. weight [g/mol]: 321.37

Physical Properties

Property code	Value	Unit	Source
gf	-220.26	kJ/mol	Joback Method
hf	-637.03	kJ/mol	Joback Method
hfus	41.59	kJ/mol	Joback Method
hvap	83.76	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	1.870		Crippen Method
mcvol	253.060	ml/mol	McGowan Method
pc	1734.67	kPa	Joback Method
rinpol	2694.00		NIST Webbook
rinpol	2694.00		NIST Webbook
tb	853.89	K	Joback Method
tc	1065.03	K	Joback Method
tf	531.94	K	Joback Method
vc	0.955	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.34	J/mol×K	853.89	Joback Method
cpg	776.09	J/mol×K	889.08	Joback Method
cpg	788.72	J/mol×K	924.27	Joback Method
cpg	800.24	J/mol×K	959.46	Joback Method
cpg	810.66	J/mol×K	994.65	Joback Method
cpg	820.00	J/mol×K	1029.84	Joback Method
cpg	828.26	J/mol×K	1065.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357530&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
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