Fumaric acid, monoamide, N-(3,4-dimethoxyphenethyl)-, 2-pentyl ester

Inchi: InChI=1S/C19H27NO5/c1-5-6-14(2)25-19(22)10-9-18(21)20-12-11-15-7-8-16(23-3)17(13

InchiKey: HYIPBMWXRKMMNI-MDZDMXLPSA-N

Formula: C19H27NO5

SMILES: CCCC(C)OC(=O)C=CC(=O)NCCc1ccc(OC)c(OC)c1

Mol. weight [g/mol]: 349.42

Physical Properties

Property code	Value	Unit	Source
gf	-203.42	kJ/mol	Joback Method
hf	-678.31	kJ/mol	Joback Method
hfus	46.77	kJ/mol	Joback Method
hvap	88.22	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	2.650		Crippen Method
mcvol	281.240	ml/mol	McGowan Method
pc	1487.29	kPa	Joback Method
rinpol	2931.00		NIST Webbook
tb	899.65	K	Joback Method
tc	1111.23	K	Joback Method
tf	554.48	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.39	J/mol×K	899.65	Joback Method
cpg	892.49	J/mol×K	934.91	Joback Method
cpg	905.37	J/mol×K	970.18	Joback Method
cpg	917.06	J/mol×K	1005.44	Joback Method
cpg	927.57	J/mol×K	1040.70	Joback Method
cpg	936.91	J/mol×K	1075.97	Joback Method
cpg	945.11	J/mol×K	1111.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357502&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
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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