

Fumaric acid, monoamide, N-(3,4-dimethoxyphenethyl)-, 3,5-difluorophenyl ester

Other names:	Fumaric acid, monoamide, N-(3,4-dimethoxyphenethyl)-, 3,5-fluorophenyl ester
Inchi:	InChI=1S/C20H19F2NO5/c1-26-17-4-3-13(9-18(17)27-2)7-8-23-19(24)5-6-20(25)28-16-1
InchiKey:	DYYPBHAKVSVGSJ-AATRIKPKSA-N
Formula:	C20H19F2NO5
SMILES:	COc1ccc(CCNC(=O)C=CC(=O)Oc2cc(F)cc(F)c2)cc1OC
Mol. weight [g/mol]:	391.37

Physical Properties

Property code	Value	Unit	Source
gf	-489.03	kJ/mol	Joback Method
hf	-872.30	kJ/mol	Joback Method
hfus	52.30	kJ/mol	Joback Method
hvap	92.80	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	2.802		Crippen Method
mcvol	275.110	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	3114.00		NIST Webbook
tb	958.15	K	Joback Method
tc	1181.76	K	Joback Method
tf	633.39	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.81	J/molxK	958.15	Joback Method
cpg	854.67	J/molxK	995.42	Joback Method
cpg	864.27	J/molxK	1032.69	Joback Method
cpg	872.60	J/molxK	1069.95	Joback Method
cpg	879.70	J/molxK	1107.22	Joback Method
cpg	885.58	J/molxK	1144.49	Joback Method
cpg	890.27	J/molxK	1181.76	Joback Method

Sources

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=U357412&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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