

Fumaric acid, monoamide, N,N-dimethyl-, 3,5-difluorophenyl ester

Other names:	Fumaric acid, monoamide, N,N-dimethyl-, 3,5-fluorophenyl ester
Inchi:	InChI=1S/C12H11F2NO3/c1-15(2)11(16)3-4-12(17)18-10-6-8(13)5-9(14)7-10/h3-7H,1-2H
InchiKey:	YQVPTQXBHROYMX-ONEGZZNKSA-N
Formula:	C12H11F2NO3
SMILES:	CN(C)C(=O)C=CC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]:	255.22

Physical Properties

Property code	Value	Unit	Source
gf	-418.15	kJ/mol	Joback Method
hf	-642.27	kJ/mol	Joback Method
hfus	33.87	kJ/mol	Joback Method
hvap	62.17	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	1.515		Crippen Method
mcvol	174.410	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	1911.00		NIST Webbook
rinpol	1911.00		NIST Webbook
tb	655.90	K	Joback Method
tc	858.15	K	Joback Method
tf	427.12	K	Joback Method
vc	0.663	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.02	J/mol×K	655.90	Joback Method
cpg	453.98	J/mol×K	689.61	Joback Method
cpg	465.17	J/mol×K	723.32	Joback Method
cpg	475.63	J/mol×K	757.02	Joback Method
cpg	485.38	J/mol×K	790.73	Joback Method
cpg	494.45	J/mol×K	824.44	Joback Method
cpg	502.88	J/mol×K	858.15	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=U357404&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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