

Fumaric acid, monoamide, N-methyl-N-phenyl-, 3,5-difluorophenyl ester

Other names:	Fumaric acid, monoamide, N-methyl-N-phenyl-, 3,5-fluorophenyl ester
Inchi:	InChI=1S/C17H13F2NO3/c1-20(14-5-3-2-4-6-14)16(21)7-8-17(22)23-15-10-12(18)9-13(19)
InchiKey:	PWQXQXKJMUZSQ-BQYQJAHWSA-N
Formula:	C17H13F2NO3
SMILES:	CN(C(=O)C=CC(=O)Oc1cc(F)cc(F)c1)c1ccccc1
Mol. weight [g/mol]:	317.29

Physical Properties

Property code	Value	Unit	Source
gf	-263.64	kJ/mol	Joback Method
hf	-508.94	kJ/mol	Joback Method
hfus	40.86	kJ/mol	Joback Method
hvap	75.58	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.089		Crippen Method
mcvol	221.100	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	2343.00		NIST Webbook
tb	796.98	K	Joback Method
tc	1019.81	K	Joback Method
tf	509.89	K	Joback Method
vc	0.836	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.77	J/molxK	796.98	Joback Method
cpg	627.24	J/molxK	834.12	Joback Method
cpg	638.68	J/molxK	871.26	Joback Method
cpg	649.17	J/molxK	908.39	Joback Method
cpg	658.77	J/molxK	945.53	Joback Method
cpg	667.54	J/molxK	982.67	Joback Method
cpg	675.55	J/molxK	1019.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357405&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
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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