Fumaric acid, monoamide, N,N-dimethyl-, 3-fluorophenyl ester

Inchi: InChI=1S/C12H12FNO3/c1-14(2)11(15)6-7-12(16)17-10-5-3-4-9(13)8-10/h3-8H,1-2H3/b7

InchiKey: VLOURVXLDFCDNF-VOTSOKGWSA-N

Formula: C12H12FNO3

SMILES: CN(C)C(=O)C=CC(=O)Oc1cccc(F)c1

Mol. weight [g/mol]: 237.23

Physical Properties

Property code	Value	Unit	Source
gf	-213.71	kJ/mol	Joback Method
hf	-434.69	kJ/mol	Joback Method
hfus	31.18	kJ/mol	Joback Method
hvap	62.33	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.375		Crippen Method
mcvol	172.640	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
tb	651.65	K	Joback Method
tc	861.81	K	Joback Method
tf	414.01	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.99	J/mol×K	651.65	Joback Method
cpg	447.71	J/mol×K	686.68	Joback Method
cpg	459.57	J/mol×K	721.70	Joback Method
cpg	470.61	J/mol×K	756.73	Joback Method
cpg	480.87	J/mol×K	791.76	Joback Method
cpg	490.40	J/mol×K	826.78	Joback Method
cpg	499.22	J/mol×K	861.81	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=U357484&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
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