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

Inchi: InChI=1S/C13H15NO3/c1-10-5-4-6-11(9-10)17-13(16)8-7-12(15)14(2)3/h4-9H,1-3H3/b8-

InchiKey: MBVABSHKNPWPMR-BQYQJAHWSA-N

Formula: C13H15NO3

SMILES: Cc1cccc(OC(=O)C=CC(=O)N(C)C)c1

Mol. weight [g/mol]: 233.26

Physical Properties

Property code	Value	Unit	Source
gf	-10.48	kJ/mol	Joback Method
hf	-259.22	kJ/mol	Joback Method
hfus	30.69	kJ/mol	Joback Method
hvap	65.37	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.545		Crippen Method
mcvol	184.960	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
rinpol	2123.00		NIST Webbook
rinpol	2123.00		NIST Webbook
tb	675.26	K	Joback Method
tc	891.30	K	Joback Method
tf	424.69	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.47	J/mol×K	675.26	Joback Method
cpg	491.36	J/mol×K	711.27	Joback Method
cpg	504.31	J/mol×K	747.27	Joback Method
cpg	516.36	J/mol×K	783.28	Joback Method
cpg	527.56	J/mol×K	819.29	Joback Method
cpg	537.95	J/mol×K	855.29	Joback Method
cpg	547.57	J/mol×K	891.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357454&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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