Fumaric acid, monoamide, N-methyl-N-phenyl-, 3,4-dimethylphenyl ester

Inchi: InChI=1S/C19H19NO3/c1-14-9-10-17(13-15(14)2)23-19(22)12-11-18(21)20(3)16-7-5-4-6

InchiKey: GPPJTWMHDWGONZ-VAWYXSNFSA-N

Formula: C19H19NO3

SMILES: Cc1ccc(OC(=O)C=CC(=O)N(C)c2ccccc2)cc1C

Mol. weight [g/mol]: 309.36

Physical Properties

Property code	Value	Unit	Source
gf	142.82	kJ/mol	Joback Method
hf	-158.00	kJ/mol	Joback Method
hfus	39.88	kJ/mol	Joback Method
hvap	81.67	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.428		Crippen Method
mcvol	245.740	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	2764.00		NIST Webbook
tb	844.20	K	Joback Method
tc	1077.17	K	Joback Method
tf	531.25	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.37	J/mol×K	844.20	Joback Method
cpg	724.50	J/mol×K	883.03	Joback Method
cpg	737.47	J/mol×K	921.86	Joback Method
cpg	749.37	J/mol×K	960.69	Joback Method
cpg	760.28	J/mol×K	999.51	Joback Method
cpg	770.28	J/mol×K	1038.34	Joback Method
cpg	779.44	J/mol×K	1077.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357431&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