Fumaric acid, monoamide, N,N-dimethyl-, 3,4-dimethylphenyl ester

Inchi: InChI=1S/C14H17NO3/c1-10-5-6-12(9-11(10)2)18-14(17)8-7-13(16)15(3)4/h5-9H,1-4H3/

InchiKey: HWVRSALFSZGLDI-BQYQJAHWSA-N

Formula: C14H17NO3

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

Mol. weight [g/mol]: 247.29

Physical Properties

Property code	Value	Unit	Source
gf	-11.69	kJ/mol	Joback Method
hf	-291.33	kJ/mol	Joback Method
hfus	32.89	kJ/mol	Joback Method
hvap	68.26	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.853		Crippen Method
mcvol	199.050	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	2286.00		NIST Webbook
rinpol	2286.00		NIST Webbook
tb	703.12	K	Joback Method
tc	916.68	K	Joback Method
tf	448.48	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.39	J/mol×K	703.12	Joback Method
cpg	542.60	J/mol×K	738.71	Joback Method
cpg	555.87	J/mol×K	774.31	Joback Method
cpg	568.26	J/mol×K	809.90	Joback Method
cpg	579.80	J/mol×K	845.49	Joback Method
cpg	590.52	J/mol×K	881.08	Joback Method
cpg	600.48	J/mol×K	916.68	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357430&Units=SI

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