Fumaric acid, monoamide, N-methyl-N-phenyl-, isopropyl ester

Inchi: InChI=1S/C14H17NO3/c1-11(2)18-14(17)10-9-13(16)15(3)12-7-5-4-6-8-12/h4-11H,1-3H3

InchiKey: WCICBBMCSVTQDS-MDZDMXLPSA-N

Formula: C14H17NO3

SMILES: CC(C)OC(=O)C=CC(=O)N(C)c1ccccc1

Mol. weight [g/mol]: 247.29

Physical Properties

Property code	Value	Unit	Source
gf	5.13	kJ/mol	Joback Method
hf	-273.67	kJ/mol	Joback Method
hfus	30.14	kJ/mol	Joback Method
hvap	66.55	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.157		Crippen Method
mcvol	199.050	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	1960.00		NIST Webbook
tb	692.72	K	Joback Method
tc	908.46	K	Joback Method
tf	408.44	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.80	J/mol×K	692.72	Joback Method
cpg	545.59	J/mol×K	728.68	Joback Method
cpg	559.34	J/mol×K	764.63	Joback Method
cpg	572.11	J/mol×K	800.59	Joback Method
cpg	583.96	J/mol×K	836.55	Joback Method
cpg	594.93	J/mol×K	872.51	Joback Method
cpg	605.08	J/mol×K	908.46	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=U357521&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