Fumaric acid, monoamide, N-methyl-N-phenyl-, 4-isopropoxyphenyl ester

Inchi: InChI=1S/C20H21NO4/c1-15(2)24-17-9-11-18(12-10-17)25-20(23)14-13-19(22)21(3)16-7

InchiKey: XCXWNDVFTXQAHX-BUHFOSPRSA-N

Formula: C20H21NO4

SMILES: CC(C)Oc1ccc(OC(=O)C=CC(=O)N(C)c2ccccc2)cc1

Mol. weight [g/mol]: 339.38

Physical Properties

Property code	Value	Unit	Source
gf	53.43	kJ/mol	Joback Method
hf	-304.67	kJ/mol	Joback Method
hfus	40.52	kJ/mol	Joback Method
hvap	85.25	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.598		Crippen Method
mcvol	265.700	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
rinpol	2731.00		NIST Webbook
rinpol	2731.00		NIST Webbook
tb	884.08	K	Joback Method
tc	1115.08	K	Joback Method
tf	537.23	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.96	J/mol×K	884.08	Joback Method
cpg	809.85	J/mol×K	922.58	Joback Method
cpg	822.49	J/mol×K	961.08	Joback Method
cpg	833.96	J/mol×K	999.58	Joback Method
cpg	844.33	J/mol×K	1038.08	Joback Method
cpg	853.67	J/mol×K	1076.58	Joback Method
cpg	862.05	J/mol×K	1115.08	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=U357421&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