Fumaric acid, monoamide, N-(4-phenoxyphenyl)-, isopropyl ester

Inchi: InChI=1S/C19H19NO4/c1-14(2)23-19(22)13-12-18(21)20-15-8-10-17(11-9-15)24-16-6-4-

InchiKey: VNZLKYTVONWSFR-OUKQBFOZSA-N

Formula: C19H19NO4

SMILES: CC(C)OC(=O)C=CC(=O)Nc1ccc(Oc2ccccc2)cc1

Mol. weight [g/mol]: 325.36

Physical Properties

Property code	Value	Unit	Source
gf	23.62	kJ/mol	Joback Method
hf	-298.09	kJ/mol	Joback Method
hfus	40.01	kJ/mol	Joback Method
hvap	87.42	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.925		Crippen Method
mcvol	251.610	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	2997.00		NIST Webbook
tb	898.93	K	Joback Method
tc	1134.47	K	Joback Method
tf	546.15	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.06	J/mol×K	898.93	Joback Method
cpg	763.79	J/mol×K	938.19	Joback Method
cpg	775.28	J/mol×K	977.44	Joback Method
cpg	785.60	J/mol×K	1016.70	Joback Method
cpg	794.81	J/mol×K	1055.96	Joback Method
cpg	802.97	J/mol×K	1095.22	Joback Method
cpg	810.14	J/mol×K	1134.47	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=U357529&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