Fumaric acid, monoamide, N-(4-phenoxyphenyl)-, 2-pentyl ester

Inchi: InChI=1S/C21H23NO4/c1-3-7-16(2)25-21(24)15-14-20(23)22-17-10-12-19(13-11-17)26-1

InchiKey: OQFBHKOZWWEKKI-CCEZHUSRSA-N

Formula: C21H23NO4

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

Mol. weight [g/mol]: 353.41

Physical Properties

Property code	Value	Unit	Source
gf	40.46	kJ/mol	Joback Method
hf	-339.37	kJ/mol	Joback Method
hfus	45.19	kJ/mol	Joback Method
hvap	91.87	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.705		Crippen Method
mcvol	279.790	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
rinpol	3214.00		NIST Webbook
tb	944.69	K	Joback Method
tc	1176.80	K	Joback Method
tf	568.69	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.41	J/mol×K	944.69	Joback Method
cpg	879.36	J/mol×K	983.37	Joback Method
cpg	891.05	J/mol×K	1022.06	Joback Method
cpg	901.57	J/mol×K	1060.74	Joback Method
cpg	910.98	J/mol×K	1099.43	Joback Method
cpg	919.34	J/mol×K	1138.11	Joback Method
cpg	926.73	J/mol×K	1176.80	Joback Method

Sources

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=U357501&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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