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

Inchi: InChI=1S/C21H23NO4/c1-21(2,3)15-25-20(24)14-13-19(23)22-16-9-11-18(12-10-16)26-1

InchiKey: SJHAZBNZUPYIBL-BUHFOSPRSA-N

Formula: C21H23NO4

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

Mol. weight [g/mol]: 353.41

Physical Properties

Property code	Value	Unit	Source
gf	45.74	kJ/mol	Joback Method
hf	-342.84	kJ/mol	Joback Method
hfus	41.30	kJ/mol	Joback Method
hvap	90.96	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.563		Crippen Method
mcvol	279.790	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	3176.00		NIST Webbook
rinpol	3176.00		NIST Webbook
tb	941.90	K	Joback Method
tc	1178.68	K	Joback Method
tf	586.11	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.51	J/mol×K	941.90	Joback Method
cpg	879.66	J/mol×K	981.36	Joback Method
cpg	891.65	J/mol×K	1020.83	Joback Method
cpg	902.57	J/mol×K	1060.29	Joback Method
cpg	912.53	J/mol×K	1099.75	Joback Method
cpg	921.62	J/mol×K	1139.21	Joback Method
cpg	929.94	J/mol×K	1178.68	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=U357519&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