Fumaric acid, monoamide, N-(2,4-dimethoxyphenyl)-, neopentyl ester

Inchi: InChI=1S/C17H23NO5/c1-17(2,3)11-23-16(20)9-8-15(19)18-13-7-6-12(21-4)10-14(13)22

InchiKey: OWSNUCOKTSZCKY-CMDGGOBGSA-N

Formula: C17H23NO5

SMILES: COc1ccc(NC(=O)C=CC(=O)OCC(C)(C)C)c(OC)c1

Mol. weight [g/mol]: 321.37

Physical Properties

Property code	Value	Unit	Source
gf	-214.98	kJ/mol	Joback Method
hf	-640.50	kJ/mol	Joback Method
hfus	37.70	kJ/mol	Joback Method
hvap	82.86	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.788		Crippen Method
mcvol	253.060	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	2709.00		NIST Webbook
rinpol	2709.00		NIST Webbook
tb	851.10	K	Joback Method
tc	1066.56	K	Joback Method
tf	549.36	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.98	J/mol×K	851.10	Joback Method
cpg	776.77	J/mol×K	887.01	Joback Method
cpg	789.45	J/mol×K	922.92	Joback Method
cpg	801.05	J/mol×K	958.83	Joback Method
cpg	811.62	J/mol×K	994.74	Joback Method
cpg	821.18	J/mol×K	1030.65	Joback Method
cpg	829.76	J/mol×K	1066.56	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=U357518&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