Fumaric acid, monoamide, N-(3,4-dimethoxyphenethyl)-, neopentyl ester

Inchi: InChI=1S/C19H27NO5/c1-19(2,3)13-25-18(22)9-8-17(21)20-11-10-14-6-7-15(23-4)16(12

InchiKey: FRRJGWIHBFHMAM-CMDGGOBGSA-N

Formula: C19H27NO5

SMILES: COc1ccc(CCNC(=O)C=CC(=O)OCC(C)(C)C)cc1OC

Mol. weight [g/mol]: 349.42

Physical Properties

Property code	Value	Unit	Source
gf	-198.14	kJ/mol	Joback Method
hf	-681.78	kJ/mol	Joback Method
hfus	42.88	kJ/mol	Joback Method
hvap	87.31	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.508		Crippen Method
mcvol	281.240	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	2847.00		NIST Webbook
rinpol	2847.00		NIST Webbook
tb	896.86	K	Joback Method
tc	1111.45	K	Joback Method
tf	571.90	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.59	J/mol×K	896.86	Joback Method
cpg	892.74	J/mol×K	932.63	Joback Method
cpg	905.73	J/mol×K	968.39	Joback Method
cpg	917.58	J/mol×K	1004.16	Joback Method
cpg	928.36	J/mol×K	1039.92	Joback Method
cpg	938.08	J/mol×K	1075.69	Joback Method
cpg	946.78	J/mol×K	1111.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357520&Units=SI
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

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