Fumaric acid, monoamide, N-(3,4-dimethoxyphenethyl)-, 2-ethylhexyl ester

Inchi: InChI=1S/C22H33NO5/c1-5-7-8-17(6-2)16-28-22(25)12-11-21(24)23-14-13-18-9-10-19(2

InchiKey: FYFOFPIFRFAAMA-VAWYXSNFSA-N

Formula: C22H33NO5

SMILES: CCCCC(CC)COC(=O)C=CC(=O)NCCc1ccc(OC)c(OC)c1

Mol. weight [g/mol]: 391.50

Physical Properties

Property code	Value	Unit	Source
gf	-178.16	kJ/mol	Joback Method
hf	-740.23	kJ/mol	Joback Method
hfus	54.54	kJ/mol	Joback Method
hvap	94.89	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	3.678		Crippen Method
mcvol	323.510	ml/mol	McGowan Method
pc	1204.80	kPa	Joback Method
rinpol	3274.00		NIST Webbook
rinpol	3274.00		NIST Webbook
tb	968.29	K	Joback Method
tc	1186.61	K	Joback Method
tf	588.29	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.34	J/mol×K	968.29	Joback Method
cpg	1071.90	J/mol×K	1004.68	Joback Method
cpg	1085.05	J/mol×K	1041.06	Joback Method
cpg	1096.82	J/mol×K	1077.45	Joback Method
cpg	1107.25	J/mol×K	1113.84	Joback Method
cpg	1116.36	J/mol×K	1150.23	Joback Method
cpg	1124.19	J/mol×K	1186.61	Joback Method

Sources

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=U357511&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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