Benzamide, 3,4-dimethoxy-N-(2-ethylhexyl)-

Inchi: InChI=1S/C17H27NO3/c1-5-7-8-13(6-2)12-18-17(19)14-9-10-15(20-3)16(11-14)21-4/h9-1
InchiKey: KUIUXGMVTJBCSQ-UHFFFAOYSA-N
Formula: C17H27NO3
SMILES: CCCCC(CC)CNC(=O)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 293.40

Physical Properties

Property code	Value	Unit	Source
gf	-66.56	kJ/mol	Joback Method
hf	-509.45	kJ/mol	Joback Method
hfus	38.60	kJ/mol	Joback Method
hvap	74.65	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.650		Crippen Method
mcvol	249.920	ml/mol	McGowan Method
pc	1601.28	kPa	Joback Method
rinpol	2453.00		NIST Webbook
rinpol	2453.00		NIST Webbook
tb	773.44	K	Joback Method
tc	972.50	K	Joback Method
tf	464.86	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.19	J/mol×K	773.44	Joback Method
cpg	759.61	J/mol×K	806.62	Joback Method
cpg	775.00	J/mol×K	839.79	Joback Method
cpg	789.37	J/mol×K	872.97	Joback Method
cpg	802.74	J/mol×K	906.14	Joback Method
cpg	815.11	J/mol×K	939.32	Joback Method
cpg	826.50	J/mol×K	972.50	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=U408007&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