Benzamide, 3,4-dimethoxy-N-butyl-

Inchi: InChI=1S/C13H19NO3/c1-4-5-8-14-13(15)10-6-7-11(16-2)12(9-10)17-3/h6-7,9H,4-5,8H2
InchiKey: KEBWOOMKEMSTRE-UHFFFAOYSA-N
Formula: C13H19NO3
SMILES: CCCCNC(=O)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 237.29

Physical Properties

Property code	Value	Unit	Source
gf	-97.80	kJ/mol	Joback Method
hf	-421.61	kJ/mol	Joback Method
hfus	31.76	kJ/mol	Joback Method
hvap	66.13	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.234		Crippen Method
mcvol	193.560	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook
tb	682.36	K	Joback Method
tc	885.46	K	Joback Method
tf	434.78	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.52	J/mol×K	682.36	Joback Method
cpg	537.27	J/mol×K	716.21	Joback Method
cpg	551.19	J/mol×K	750.06	Joback Method
cpg	564.27	J/mol×K	783.91	Joback Method
cpg	576.52	J/mol×K	817.76	Joback Method
cpg	587.94	J/mol×K	851.61	Joback Method
cpg	598.54	J/mol×K	885.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U408002&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