Benzamide, 3,4-dimethoxy-N-octyl-

Inchi: InChI=1S/C17H27NO3/c1-4-5-6-7-8-9-12-18-17(19)14-10-11-15(20-2)16(13-14)21-3/h10
InchiKey: PPCZRRYXPYAMEM-UHFFFAOYSA-N
Formula: C17H27NO3
SMILES: CCCCCCCCNC(=O)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 293.40

Physical Properties

Property code	Value	Unit	Source
gf	-64.12	kJ/mol	Joback Method
hf	-504.17	kJ/mol	Joback Method
hfus	42.12	kJ/mol	Joback Method
hvap	75.04	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.794		Crippen Method
mcvol	249.920	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	2563.00		NIST Webbook
rinpol	2563.00		NIST Webbook
tb	773.88	K	Joback Method
tc	970.50	K	Joback Method
tf	479.86	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.66	J/mol×K	773.88	Joback Method
cpg	758.88	J/mol×K	806.65	Joback Method
cpg	774.10	J/mol×K	839.42	Joback Method
cpg	788.33	J/mol×K	872.19	Joback Method
cpg	801.59	J/mol×K	904.96	Joback Method
cpg	813.90	J/mol×K	937.73	Joback Method
cpg	825.25	J/mol×K	970.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U408009&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

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