Benzamide, 3,4-dimethoxy-N-pentyl-

Inchi: InChI=1S/C14H21NO3/c1-4-5-6-9-15-14(16)11-7-8-12(17-2)13(10-11)18-3/h7-8,10H,4-6
InchiKey: BHFYVOLTMPOZLL-UHFFFAOYSA-N
Formula: C14H21NO3
SMILES: CCCCCNC(=O)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 251.32

Physical Properties

Property code	Value	Unit	Source
gf	-89.38	kJ/mol	Joback Method
hf	-442.25	kJ/mol	Joback Method
hfus	34.35	kJ/mol	Joback Method
hvap	68.36	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.624		Crippen Method
mcvol	207.650	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	2253.00		NIST Webbook
rinpol	2253.00		NIST Webbook
tb	705.24	K	Joback Method
tc	906.02	K	Joback Method
tf	446.05	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.79	J/mol×K	705.24	Joback Method
cpg	590.99	J/mol×K	738.70	Joback Method
cpg	605.31	J/mol×K	772.17	Joback Method
cpg	618.77	J/mol×K	805.63	Joback Method
cpg	631.35	J/mol×K	839.10	Joback Method
cpg	643.07	J/mol×K	872.56	Joback Method
cpg	653.93	J/mol×K	906.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U408004&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