Benzamide, 3,4-dimethoxy-N-(3-methylbutyl)-

Inchi: InChI=1S/C14H21NO3/c1-10(2)7-8-15-14(16)11-5-6-12(17-3)13(9-11)18-4/h5-6,9-10H,7-
InchiKey: CNUHWGYPQRLXGA-UHFFFAOYSA-N
Formula: C14H21NO3
SMILES: COc1ccc(C(=O)NCCC(C)C)cc1OC
Mol. weight [g/mol]: 251.32

Physical Properties

Property code	Value	Unit	Source
gf	-91.82	kJ/mol	Joback Method
hf	-447.53	kJ/mol	Joback Method
hfus	30.83	kJ/mol	Joback Method
hvap	67.97	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.480		Crippen Method
mcvol	207.650	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook
tb	704.80	K	Joback Method
tc	908.86	K	Joback Method
tf	431.05	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.31	J/mol×K	704.80	Joback Method
cpg	591.78	J/mol×K	738.81	Joback Method
cpg	606.34	J/mol×K	772.82	Joback Method
cpg	619.98	J/mol×K	806.83	Joback Method
cpg	632.72	J/mol×K	840.84	Joback Method
cpg	644.55	J/mol×K	874.85	Joback Method
cpg	655.50	J/mol×K	908.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U408003&Units=SI

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