

Benzanilide,3',4',5'-trimethoxy-2-methylamino-

Inchi:	InChI=1S/C17H20N2O4/c1-18-13-8-6-5-7-12(13)17(20)19-11-9-14(21-2)16(23-4)15(10-1
InchiKey:	BJIUTMDVMUBADL-UHFFFAOYSA-N
Formula:	C17H20N2O4
SMILES:	CNc1ccccc1C(=O)Nc1cc(OC)c(OC)c(OC)c1
Mol. weight [g/mol]:	316.35
CAS:	1043-91-0

Physical Properties

Property code	Value	Unit	Source
gf	13.42	kJ/mol	Joback Method
hf	-369.33	kJ/mol	Joback Method
hfus	41.67	kJ/mol	Joback Method
hvap	87.48	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.006		Crippen Method
mcvol	242.010	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
tb	883.11	K	Joback Method
tc	1109.22	K	Joback Method
tf	606.21	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.22	J/mol×K	883.11	Joback Method
cpg	742.98	J/mol×K	920.79	Joback Method
cpg	754.41	J/mol×K	958.48	Joback Method
cpg	764.51	J/mol×K	996.16	Joback Method
cpg	773.27	J/mol×K	1033.85	Joback Method
cpg	780.69	J/mol×K	1071.53	Joback Method
cpg	786.76	J/mol×K	1109.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1043910&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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