Benzamide, 3-methoxy-N-(3-methoxybenzoyl)-N-butyl-

Inchi: InChI=1S/C20H23NO4/c1-4-5-12-21(19(22)15-8-6-10-17(13-15)24-2)20(23)16-9-7-11-18

InchiKey: XCMLAVMKMUXMBQ-UHFFFAOYSA-N

Formula: C20H23NO4

SMILES: CCCCN(C(=O)c1cccc(OC)c1)C(=O)c1cccc(OC)c1

Mol. weight [g/mol]: 341.40

Physical Properties

Property code	Value	Unit	Source
gf	-33.98	kJ/mol	Joback Method
hf	-428.08	kJ/mol	Joback Method
hfus	43.45	kJ/mol	Joback Method
hvap	86.34	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	3.786		Crippen Method
mcvol	270.000	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	2607.00		NIST Webbook
rinpol	2607.00		NIST Webbook
tb	885.34	K	Joback Method
tc	1108.34	K	Joback Method
tf	569.83	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.91	J/mol×K	885.34	Joback Method
cpg	835.93	J/mol×K	922.51	Joback Method
cpg	848.66	J/mol×K	959.67	Joback Method
cpg	860.16	J/mol×K	996.84	Joback Method
cpg	870.46	J/mol×K	1034.01	Joback Method
cpg	879.60	J/mol×K	1071.18	Joback Method
cpg	887.63	J/mol×K	1108.34	Joback Method

Sources

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=U407525&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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