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

Inchi: InChI=1S/C19H21NO4/c1-4-11-20(18(21)14-7-5-9-16(12-14)23-2)19(22)15-8-6-10-17(13

InchiKey: GTECBACKLSNTSX-UHFFFAOYSA-N

Formula: C19H21NO4

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

Mol. weight [g/mol]: 327.37

Physical Properties

Property code	Value	Unit	Source
gf	-42.40	kJ/mol	Joback Method
hf	-407.44	kJ/mol	Joback Method
hfus	40.86	kJ/mol	Joback Method
hvap	84.12	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.396		Crippen Method
mcvol	255.910	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	2478.00		NIST Webbook
rinpol	2478.00		NIST Webbook
tb	862.46	K	Joback Method
tc	1087.09	K	Joback Method
tf	558.56	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.42	J/mol×K	862.46	Joback Method
cpg	778.35	J/mol×K	899.90	Joback Method
cpg	791.02	J/mol×K	937.34	Joback Method
cpg	802.46	J/mol×K	974.77	Joback Method
cpg	812.71	J/mol×K	1012.21	Joback Method
cpg	821.81	J/mol×K	1049.65	Joback Method
cpg	829.81	J/mol×K	1087.09	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=U407523&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

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