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

Inchi: InChI=1S/C21H25NO4/c1-15(2)11-12-22(20(23)16-7-5-9-18(13-16)25-3)21(24)17-8-6-10

InchiKey: DQGYPEDORNYBFQ-UHFFFAOYSA-N

Formula: C21H25NO4

SMILES: COc1cccc(C(=O)N(CCC(C)C)C(=O)c2cccc(OC)c2)c1

Mol. weight [g/mol]: 355.43

Physical Properties

Property code	Value	Unit	Source
gf	-28.00	kJ/mol	Joback Method
hf	-454.00	kJ/mol	Joback Method
hfus	42.52	kJ/mol	Joback Method
hvap	88.18	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.032		Crippen Method
mcvol	284.090	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	2655.00		NIST Webbook
rinpol	2655.00		NIST Webbook
tb	907.78	K	Joback Method
tc	1132.21	K	Joback Method
tf	566.10	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.61	J/mol×K	907.78	Joback Method
cpg	894.81	J/mol×K	945.19	Joback Method
cpg	907.67	J/mol×K	982.59	Joback Method
cpg	919.23	J/mol×K	1020.00	Joback Method
cpg	929.54	J/mol×K	1057.40	Joback Method
cpg	938.65	J/mol×K	1094.81	Joback Method
cpg	946.60	J/mol×K	1132.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407526&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume