Benzamide, N-(2,5-dimethoxyphenyl)-4-butyl-

Inchi: InChI=1S/C19H23NO3/c1-4-5-6-14-7-9-15(10-8-14)19(21)20-17-13-16(22-2)11-12-18(17
InchiKey: DQEJZNNSDCHGBN-UHFFFAOYSA-N
Formula: C19H23NO3
SMILES: CCCCc1ccc(C(=O)Nc2cc(OC)ccc2OC)cc1
Mol. weight [g/mol]: 313.39

Physical Properties

Property code	Value	Unit	Source
gf	55.50	kJ/mol	Joback Method
hf	-320.39	kJ/mol	Joback Method
hfus	40.95	kJ/mol	Joback Method
hvap	82.43	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.299		Crippen Method
mcvol	254.340	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2772.00		NIST Webbook
rinpol	2772.00		NIST Webbook
tb	851.30	K	Joback Method
tc	1073.19	K	Joback Method
tf	541.34	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.05	J/mol×K	851.30	Joback Method
cpg	778.91	J/mol×K	888.28	Joback Method
cpg	792.51	J/mol×K	925.26	Joback Method
cpg	804.89	J/mol×K	962.24	Joback Method
cpg	816.07	J/mol×K	999.23	Joback Method
cpg	826.07	J/mol×K	1036.21	Joback Method
cpg	834.92	J/mol×K	1073.19	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=U306995&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