Benzamide, N-(4-methoxyphenyl)-4-butyl-

Inchi: InChI=1S/C18H21NO2/c1-3-4-5-14-6-8-15(9-7-14)18(20)19-16-10-12-17(21-2)13-11-16/h
InchiKey: DMPZYHAVRAVWJR-UHFFFAOYSA-N
Formula: C18H21NO2
SMILES: CCCCc1ccc(C(=O)Nc2ccc(OC)cc2)cc1
Mol. weight [g/mol]: 283.36

Physical Properties

Property code	Value	Unit	Source
gf	161.71	kJ/mol	Joback Method
hf	-156.06	kJ/mol	Joback Method
hfus	37.57	kJ/mol	Joback Method
hvap	77.13	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.290		Crippen Method
mcvol	234.380	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	2676.00		NIST Webbook
tb	801.02	K	Joback Method
tc	1026.27	K	Joback Method
tf	495.32	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.59	J/mol×K	801.02	Joback Method
cpg	696.00	J/mol×K	838.56	Joback Method
cpg	710.21	J/mol×K	876.10	Joback Method
cpg	723.27	J/mol×K	913.64	Joback Method
cpg	735.24	J/mol×K	951.19	Joback Method
cpg	746.16	J/mol×K	988.73	Joback Method
cpg	756.08	J/mol×K	1026.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306993&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

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