Benzamide, 4-methoxy-N-butyl-N-hept-2-yl-

Inchi: InChI=1S/C19H31NO2/c1-6-8-14-20(18(9-7-2)15(3)4)19(21)16-10-12-17(22-5)13-11-16/h
InchiKey: LSTYWSHHPIKXFL-UHFFFAOYSA-N
Formula: C19H31NO2
SMILES: CCCCN(C(=O)c1ccc(OC)cc1)C(CCC)C(C)C
Mol. weight [g/mol]: 305.45

Physical Properties

Property code	Value	Unit	Source
gf	83.86	kJ/mol	Joback Method
hf	-398.26	kJ/mol	Joback Method
hfus	37.38	kJ/mol	Joback Method
hvap	71.25	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.762		Crippen Method
mcvol	272.230	ml/mol	McGowan Method
pc	1406.95	kPa	Joback Method
rinpol	2839.00		NIST Webbook
rinpol	2839.00		NIST Webbook
tb	753.63	K	Joback Method
tc	949.37	K	Joback Method
tf	417.46	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	810.69	J/mol×K	753.63	Joback Method
cpg	829.17	J/mol×K	786.25	Joback Method
cpg	846.53	J/mol×K	818.88	Joback Method
cpg	862.83	J/mol×K	851.50	Joback Method
cpg	878.10	J/mol×K	884.12	Joback Method
cpg	892.38	J/mol×K	916.74	Joback Method
cpg	905.71	J/mol×K	949.37	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=U415908&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