Benzamide, 4-methoxy-N-butyl-N-heptyl-

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

Physical Properties

Property code	Value	Unit	Source
gf	88.74	kJ/mol	Joback Method
hf	-387.70	kJ/mol	Joback Method
hfus	44.43	kJ/mol	Joback Method
hvap	72.03	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.908		Crippen Method
mcvol	272.230	ml/mol	McGowan Method
pc	1390.22	kPa	Joback Method
rinpol	3048.00		NIST Webbook
rinpol	3048.00		NIST Webbook
tb	754.51	K	Joback Method
tc	945.46	K	Joback Method
tf	447.46	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.71	J/mol×K	754.51	Joback Method
cpg	827.71	J/mol×K	786.33	Joback Method
cpg	844.67	J/mol×K	818.16	Joback Method
cpg	860.63	J/mol×K	849.98	Joback Method
cpg	875.63	J/mol×K	881.81	Joback Method
cpg	889.71	J/mol×K	913.63	Joback Method
cpg	902.90	J/mol×K	945.46	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=U415911&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