Benzamide, 4-methoxy-N-butyl-N-pentyl-

Inchi: InChI=1S/C17H27NO2/c1-4-6-8-14-18(13-7-5-2)17(19)15-9-11-16(20-3)12-10-15/h9-12H
InchiKey: YTIAKRZBEJEQKN-UHFFFAOYSA-N
Formula: C17H27NO2
SMILES: CCCCCN(CCCC)C(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 277.40

Physical Properties

Property code	Value	Unit	Source
gf	71.90	kJ/mol	Joback Method
hf	-346.42	kJ/mol	Joback Method
hfus	39.25	kJ/mol	Joback Method
hvap	67.57	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.128		Crippen Method
mcvol	244.050	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	2706.00		NIST Webbook
rinpol	2706.00		NIST Webbook
tb	708.75	K	Joback Method
tc	901.43	K	Joback Method
tf	424.92	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.28	J/mol×K	708.75	Joback Method
cpg	712.76	J/mol×K	740.86	Joback Method
cpg	729.25	J/mol×K	772.98	Joback Method
cpg	744.78	J/mol×K	805.09	Joback Method
cpg	759.38	J/mol×K	837.20	Joback Method
cpg	773.09	J/mol×K	869.32	Joback Method
cpg	785.94	J/mol×K	901.43	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=U415907&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