Benzamide, 4-methoxy-N-butyl-N-3-methylbutyl-

Inchi: InChI=1S/C17H27NO2/c1-5-6-12-18(13-11-14(2)3)17(19)15-7-9-16(20-4)10-8-15/h7-10,1

InchiKey: FXZQGTFVDVSDBT-UHFFFAOYSA-N

Formula: C17H27NO2

SMILES: CCCCN(CCC(C)C)C(=O)c1ccc(OC)cc1

Mol. weight [g/mol]: 277.40

Physical Properties

Property code	Value	Unit	Source
gf	69.46	kJ/mol	Joback Method
hf	-351.70	kJ/mol	Joback Method
hfus	35.72	kJ/mol	Joback Method
hvap	67.19	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.984		Crippen Method
mcvol	244.050	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	2720.00		NIST Webbook
rinpol	2720.00		NIST Webbook
tb	708.31	K	Joback Method
tc	903.86	K	Joback Method
tf	409.92	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.76	J/mol×K	708.31	Joback Method
cpg	713.53	J/mol×K	740.90	Joback Method
cpg	730.26	J/mol×K	773.49	Joback Method
cpg	745.99	J/mol×K	806.09	Joback Method
cpg	760.77	J/mol×K	838.68	Joback Method
cpg	774.61	J/mol×K	871.27	Joback Method
cpg	787.57	J/mol×K	903.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415906&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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