Benzamide, 4-methoxy-N-butyl-N-isobutyl-

Inchi: InChI=1S/C16H25NO2/c1-5-6-11-17(12-13(2)3)16(18)14-7-9-15(19-4)10-8-14/h7-10,13H
InchiKey: BCTIXKNNONJSLO-UHFFFAOYSA-N
Formula: C16H25NO2
SMILES: CCCCN(CC(C)C)C(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 263.38

Physical Properties

Property code	Value	Unit	Source
gf	61.04	kJ/mol	Joback Method
hf	-331.06	kJ/mol	Joback Method
hfus	33.13	kJ/mol	Joback Method
hvap	64.96	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.593		Crippen Method
mcvol	229.960	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	2480.00		NIST Webbook
rinpol	2480.00		NIST Webbook
tb	685.43	K	Joback Method
tc	882.83	K	Joback Method
tf	398.65	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.18	J/mol×K	685.43	Joback Method
cpg	657.66	J/mol×K	718.33	Joback Method
cpg	674.14	J/mol×K	751.23	Joback Method
cpg	689.63	J/mol×K	784.13	Joback Method
cpg	704.17	J/mol×K	817.03	Joback Method
cpg	717.81	J/mol×K	849.93	Joback Method
cpg	730.56	J/mol×K	882.83	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=U415904&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