Benzamide, N,N-dibutyl-3-methoxy-

Inchi: InChI=1S/C16H25NO2/c1-4-6-11-17(12-7-5-2)16(18)14-9-8-10-15(13-14)19-3/h8-10,13H
InchiKey: CLNMKRDBYLYJDD-UHFFFAOYSA-N
Formula: C16H25NO2
SMILES: CCCCN(CCCC)C(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 263.38

Physical Properties

Property code	Value	Unit	Source
gf	63.48	kJ/mol	Joback Method
hf	-325.78	kJ/mol	Joback Method
hfus	36.66	kJ/mol	Joback Method
hvap	65.35	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.738		Crippen Method
mcvol	229.960	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	2001.00		NIST Webbook
rinpol	2001.00		NIST Webbook
tb	685.87	K	Joback Method
tc	880.13	K	Joback Method
tf	413.65	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.71	J/mol×K	685.87	Joback Method
cpg	656.89	J/mol×K	718.25	Joback Method
cpg	673.09	J/mol×K	750.62	Joback Method
cpg	688.36	J/mol×K	783.00	Joback Method
cpg	702.72	J/mol×K	815.37	Joback Method
cpg	716.20	J/mol×K	847.75	Joback Method
cpg	728.83	J/mol×K	880.13	Joback Method

Sources

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=U308147&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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