Benzamide, 3-methoxy-N-octyl-

Inchi: InChI=1S/C16H25NO2/c1-3-4-5-6-7-8-12-17-16(18)14-10-9-11-15(13-14)19-2/h9-11,13H
InchiKey: IMVLBOBXWQWSPP-UHFFFAOYSA-N
Formula: C16H25NO2
SMILES: CCCCCCCCNC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 263.38

Physical Properties

Property code	Value	Unit	Source
gf	42.09	kJ/mol	Joback Method
hf	-339.84	kJ/mol	Joback Method
hfus	38.73	kJ/mol	Joback Method
hvap	69.74	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	3.785		Crippen Method
mcvol	229.960	ml/mol	McGowan Method
pc	1766.90	kPa	Joback Method
rinpol	2332.00		NIST Webbook
rinpol	2332.00		NIST Webbook
tb	723.60	K	Joback Method
tc	920.93	K	Joback Method
tf	433.84	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.90	J/mol×K	723.60	Joback Method
cpg	674.29	J/mol×K	756.49	Joback Method
cpg	689.72	J/mol×K	789.38	Joback Method
cpg	704.22	J/mol×K	822.27	Joback Method
cpg	717.82	J/mol×K	855.16	Joback Method
cpg	730.54	J/mol×K	888.04	Joback Method
cpg	742.41	J/mol×K	920.93	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=U407516&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