Benzamide, N-heptyl-N-octyl-3-methoxy-

Inchi: InChI=1S/C23H39NO2/c1-4-6-8-10-12-14-19-24(18-13-11-9-7-5-2)23(25)21-16-15-17-22
InchiKey: WQYJKKTVDPIYGW-UHFFFAOYSA-N
Formula: C23H39NO2
SMILES: CCCCCCCCN(CCCCCCC)C(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 361.56

Physical Properties

Property code	Value	Unit	Source
gf	122.42	kJ/mol	Joback Method
hf	-470.26	kJ/mol	Joback Method
hfus	54.79	kJ/mol	Joback Method
hvap	80.93	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.468		Crippen Method
mcvol	328.590	ml/mol	McGowan Method
pc	1063.79	kPa	Joback Method
rinpol	2673.00		NIST Webbook
rinpol	2673.00		NIST Webbook
tb	846.03	K	Joback Method
tc	1040.58	K	Joback Method
tf	492.54	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1049.63	J/mol×K	846.03	Joback Method
cpg	1068.62	J/mol×K	878.46	Joback Method
cpg	1086.46	J/mol×K	910.88	Joback Method
cpg	1103.18	J/mol×K	943.31	Joback Method
cpg	1118.85	J/mol×K	975.73	Joback Method
cpg	1133.50	J/mol×K	1008.16	Joback Method
cpg	1147.18	J/mol×K	1040.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308153&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