Benzamide, N,N-diheptyl-3-methoxy-

Inchi: InChI=1S/C22H37NO2/c1-4-6-8-10-12-17-23(18-13-11-9-7-5-2)22(24)20-15-14-16-21(19
InchiKey: OWALFLLYCMMSTC-UHFFFAOYSA-N
Formula: C22H37NO2
SMILES: CCCCCCCN(CCCCCCC)C(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 347.53

Physical Properties

Property code	Value	Unit	Source
gf	114.00	kJ/mol	Joback Method
hf	-449.62	kJ/mol	Joback Method
hfus	52.20	kJ/mol	Joback Method
hvap	78.70	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.078		Crippen Method
mcvol	314.500	ml/mol	McGowan Method
pc	1133.67	kPa	Joback Method
rinpol	2576.00		NIST Webbook
tb	823.15	K	Joback Method
tc	1015.79	K	Joback Method
tf	481.27	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.44	J/mol×K	823.15	Joback Method
cpg	1007.16	J/mol×K	855.26	Joback Method
cpg	1024.77	J/mol×K	887.36	Joback Method
cpg	1041.29	J/mol×K	919.47	Joback Method
cpg	1056.79	J/mol×K	951.57	Joback Method
cpg	1071.30	J/mol×K	983.68	Joback Method
cpg	1084.87	J/mol×K	1015.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308152&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