Benzamide, N,N-dihexyl-3-methoxy-

Inchi: InChI=1S/C20H33NO2/c1-4-6-8-10-15-21(16-11-9-7-5-2)20(22)18-13-12-14-19(17-18)23
InchiKey: RZDYLOFIXOHVMZ-UHFFFAOYSA-N
Formula: C20H33NO2
SMILES: CCCCCCN(CCCCCC)C(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 319.48

Physical Properties

Property code	Value	Unit	Source
gf	97.16	kJ/mol	Joback Method
hf	-408.34	kJ/mol	Joback Method
hfus	47.02	kJ/mol	Joback Method
hvap	74.25	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.298		Crippen Method
mcvol	286.320	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
rinpol	2384.00		NIST Webbook
rinpol	2384.00		NIST Webbook
tb	777.39	K	Joback Method
tc	968.28	K	Joback Method
tf	458.73	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	868.41	J/mol×K	777.39	Joback Method
cpg	886.65	J/mol×K	809.20	Joback Method
cpg	903.82	J/mol×K	841.02	Joback Method
cpg	919.98	J/mol×K	872.83	Joback Method
cpg	935.15	J/mol×K	904.65	Joback Method
cpg	949.38	J/mol×K	936.46	Joback Method
cpg	962.71	J/mol×K	968.28	Joback Method

Sources

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=U308149&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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