Benzamide, 4-methoxy-N-butyl-N-nonyl-

Inchi: InChI=1S/C21H35NO2/c1-4-6-8-9-10-11-12-18-22(17-7-5-2)21(23)19-13-15-20(24-3)16-
InchiKey: HFRRIBCTGUNMKP-UHFFFAOYSA-N
Formula: C21H35NO2
SMILES: CCCCCCCCCN(CCCC)C(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 333.51

Physical Properties

Property code	Value	Unit	Source
gf	105.58	kJ/mol	Joback Method
hf	-428.98	kJ/mol	Joback Method
hfus	49.61	kJ/mol	Joback Method
hvap	76.48	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.688		Crippen Method
mcvol	300.410	ml/mol	McGowan Method
pc	1210.67	kPa	Joback Method
rinpol	1828.00		NIST Webbook
rinpol	1828.00		NIST Webbook
tb	800.27	K	Joback Method
tc	991.70	K	Joback Method
tf	470.00	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	928.01	J/mol×K	800.27	Joback Method
cpg	946.49	J/mol×K	832.18	Joback Method
cpg	963.87	J/mol×K	864.08	Joback Method
cpg	980.21	J/mol×K	895.99	Joback Method
cpg	995.55	J/mol×K	927.89	Joback Method
cpg	1009.92	J/mol×K	959.80	Joback Method
cpg	1023.37	J/mol×K	991.70	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415913&Units=SI

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