N-Pentyl-N-methyl-benzamide

Inchi: InChI=1S/C13H19NO/c1-3-4-8-11-14(2)13(15)12-9-6-5-7-10-12/h5-7,9-10H,3-4,8,11H2,1
InchiKey: GPOLVTXJXZGYOD-UHFFFAOYSA-N
Formula: C13H19NO
SMILES: CCCCCN(C)C(=O)c1ccccc1
Mol. weight [g/mol]: 205.30

Physical Properties

Property code	Value	Unit	Source
gf	152.85	kJ/mol	Joback Method
hf	-120.17	kJ/mol	Joback Method
hfus	28.09	kJ/mol	Joback Method
hvap	55.60	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.949		Crippen Method
mcvol	181.820	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
rinpol	1724.43		NIST Webbook
rinpol	1726.78		NIST Webbook
rinpol	1747.38		NIST Webbook
rinpol	1704.11		NIST Webbook
ripol	2677.34		NIST Webbook
ripol	2656.89		NIST Webbook
ripol	2636.60		NIST Webbook
tb	589.83	K	Joback Method
tc	792.02	K	Joback Method
tf	345.09	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.79	J/mol×K	589.83	Joback Method
cpg	470.40	J/mol×K	623.53	Joback Method
cpg	486.00	J/mol×K	657.23	Joback Method

cpg	500.66	J/mol×K	690.93	Joback Method
cpg	514.41	J/mol×K	724.62	Joback Method
cpg	527.30	J/mol×K	758.32	Joback Method
cpg	539.37	J/mol×K	792.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R194151&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume