N-Hexyl-N-methyl-benzamide

Inchi: InChI=1S/C14H21NO/c1-3-4-5-9-12-15(2)14(16)13-10-7-6-8-11-13/h6-8,10-11H,3-5,9,12
InchiKey: AYXKELUADFJVAX-UHFFFAOYSA-N
Formula: C14H21NO
SMILES: CCCCCCN(C)C(=O)c1ccccc1
Mol. weight [g/mol]: 219.32

Physical Properties

Property code	Value	Unit	Source
gf	161.27	kJ/mol	Joback Method
hf	-140.81	kJ/mol	Joback Method
hfus	30.68	kJ/mol	Joback Method
hvap	57.82	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.339		Crippen Method
mcvol	195.910	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	1794.06		NIST Webbook
rinpol	1835.87		NIST Webbook
rinpol	1838.07		NIST Webbook
rinpol	1819.87		NIST Webbook
rinpol	1814.98		NIST Webbook
ripol	2747.79		NIST Webbook
ripol	2729.97		NIST Webbook
ripol	2768.83		NIST Webbook
tb	612.71	K	Joback Method
tc	812.07	K	Joback Method
tf	356.36	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.79	J/mol×K	612.71	Joback Method
cpg	521.85	J/mol×K	645.94	Joback Method

cpg	537.90	J/mol×K	679.16	Joback Method
cpg	552.98	J/mol×K	712.39	Joback Method
cpg	567.15	J/mol×K	745.62	Joback Method
cpg	580.45	J/mol×K	778.84	Joback Method
cpg	592.92	J/mol×K	812.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R194146&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume