Benzamide, 4-methyl-N-hexyl-

Inchi: InChI=1S/C14H21NO/c1-3-4-5-6-11-15-14(16)13-9-7-12(2)8-10-13/h7-10H,3-6,11H2,1-2
InchiKey: DAARZDMNSDLSQB-UHFFFAOYSA-N
Formula: C14H21NO
SMILES: CCCCCCNC(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 219.32

Physical Properties

Property code	Value	Unit	Source
gf	130.25	kJ/mol	Joback Method
hf	-166.34	kJ/mol	Joback Method
hfus	32.37	kJ/mol	Joback Method
hvap	62.88	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.305		Crippen Method
mcvol	195.910	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	1998.00		NIST Webbook
rinpol	1998.00		NIST Webbook
tb	655.42	K	Joback Method
tc	858.45	K	Joback Method
tf	389.07	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.76	J/mol×K	655.42	Joback Method
cpg	537.76	J/mol×K	689.26	Joback Method
cpg	552.84	J/mol×K	723.10	Joback Method
cpg	567.03	J/mol×K	756.94	Joback Method
cpg	580.36	J/mol×K	790.77	Joback Method
cpg	592.86	J/mol×K	824.61	Joback Method
cpg	604.59	J/mol×K	858.45	Joback Method

Sources

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=U407470&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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