

N-cyclopentyl-N-methyl-benzamide

Inchi:	InChI=1S/C13H17NO/c1-14(12-9-5-6-10-12)13(15)11-7-3-2-4-8-11/h2-4,7-8,12H,5-6,9-1
InchiKey:	WCCLGXCDZIRGLF-UHFFFAOYSA-N
Formula:	C13H17NO
SMILES:	CN(C(=O)c1ccccc1)C1CCCC1
Mol. weight [g/mol]:	203.28

Physical Properties

Property code	Value	Unit	Source
gf	189.40	kJ/mol	Joback Method
hf	-59.69	kJ/mol	Joback Method
hfus	22.02	kJ/mol	Joback Method
hvap	55.85	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.701		Crippen Method
mcvol	170.960	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
ripol	1797.22		NIST Webbook
ripol	1812.07		NIST Webbook
ripol	1823.58		NIST Webbook
ripol	1785.96		NIST Webbook
ripol	1785.96		NIST Webbook
ripol	2775.16		NIST Webbook
ripol	2763.70		NIST Webbook
ripol	2763.70		NIST Webbook
ripol	2786.20		NIST Webbook
tb	605.11	K	Joback Method
tc	836.75	K	Joback Method
tf	355.99	K	Joback Method
vc	0.621	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.74	J/mol×K	605.11	Joback Method

cpg	461.89	J/mol×K	643.72	Joback Method
cpg	479.61	J/mol×K	682.32	Joback Method
cpg	495.98	J/mol×K	720.93	Joback Method
cpg	511.09	J/mol×K	759.53	Joback Method
cpg	525.02	J/mol×K	798.14	Joback Method
cpg	537.85	J/mol×K	836.75	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=R194106&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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