

N-cyclohexyl-N-methyl-benzamide

Inchi:	InChI=1S/C14H19NO/c1-15(13-10-6-3-7-11-13)14(16)12-8-4-2-5-9-12/h2,4-5,8-9,13H,3,
InchiKey:	FEXMFEDEZGZZPC-UHFFFAOYSA-N
Formula:	C14H19NO
SMILES:	CN(C(=O)c1ccccc1)C1CCCCC1
Mol. weight [g/mol]:	217.31

Physical Properties

Property code	Value	Unit	Source
gf	185.72	kJ/mol	Joback Method
hf	-86.49	kJ/mol	Joback Method
hfus	22.51	kJ/mol	Joback Method
hvap	58.25	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.091		Crippen Method
mcvol	185.050	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1867.24		NIST Webbook
ripol	2845.11		NIST Webbook
tb	632.26	K	Joback Method
tc	867.07	K	Joback Method
tf	363.74	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.58	J/mol×K	632.26	Joback Method
cpg	516.99	J/mol×K	671.40	Joback Method
cpg	535.85	J/mol×K	710.53	Joback Method
cpg	553.26	J/mol×K	749.67	Joback Method
cpg	569.28	J/mol×K	788.80	Joback Method
cpg	583.99	J/mol×K	827.94	Joback Method
cpg	597.48	J/mol×K	867.07	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=R194097&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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