N-cycloheptyl-N-methyl-benzamide

Inchi: InChI=1S/C15H21NO/c1-16(14-11-7-2-3-8-12-14)15(17)13-9-5-4-6-10-13/h4-6,9-10,14H
InchiKey: VWYPFXAKGSHTSX-UHFFFAOYSA-N
Formula: C15H21NO
SMILES: CN(C(=O)c1ccccc1)C1CCCCCC1
Mol. weight [g/mol]: 231.33

Physical Properties

Property code	Value	Unit	Source
gf	182.04	kJ/mol	Joback Method
hf	-113.29	kJ/mol	Joback Method
hfus	23.00	kJ/mol	Joback Method
hvap	60.65	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.481		Crippen Method
mcvol	199.140	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1978.72		NIST Webbook
ripol	2956.19		NIST Webbook
tb	659.41	K	Joback Method
tc	897.14	K	Joback Method
tf	371.49	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.55	J/mol×K	659.41	Joback Method
cpg	574.07	J/mol×K	699.03	Joback Method
cpg	593.93	J/mol×K	738.65	Joback Method
cpg	612.20	J/mol×K	778.28	Joback Method
cpg	628.96	J/mol×K	817.90	Joback Method
cpg	644.27	J/mol×K	857.52	Joback Method
cpg	658.21	J/mol×K	897.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R194082&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