N-cyclopropyl-N-methyl-benzamide

Inchi: InChI=1S/C11H13NO/c1-12(10-7-8-10)11(13)9-5-3-2-4-6-9/h2-6,10H,7-8H2,1H3
InchiKey: YJGOXHXGSNBHRI-UHFFFAOYSA-N
Formula: C11H13NO
SMILES: CN(C(=O)c1ccccc1)C1CC1
Mol. weight [g/mol]: 175.23

Physical Properties

Property code	Value	Unit	Source
gf	196.76	kJ/mol	Joback Method
hf	-6.09	kJ/mol	Joback Method
hfus	21.04	kJ/mol	Joback Method
hvap	51.06	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	1.921		Crippen Method
mcvol	142.780	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	1590.59		NIST Webbook
rinpol	1551.89		NIST Webbook
rinpol	1578.45		NIST Webbook
rinpol	1563.80		NIST Webbook
ripol	2553.51		NIST Webbook
ripol	2541.26		NIST Webbook
ripol	2529.45		NIST Webbook
tb	550.81	K	Joback Method
tc	775.21	K	Joback Method
tf	340.49	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.10	J/mol×K	550.81	Joback Method
cpg	358.35	J/mol×K	588.21	Joback Method
cpg	373.38	J/mol×K	625.61	Joback Method

cpg	387.26	J/mol×K	663.01	Joback Method
cpg	400.09	J/mol×K	700.41	Joback Method
cpg	411.95	J/mol×K	737.81	Joback Method
cpg	422.92	J/mol×K	775.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R194111&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

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