Cyclopentanecarboxamide, N-(4-methoxyphenyl)-

Inchi: InChI=1S/C13H17NO2/c1-16-12-8-6-11(7-9-12)14-13(15)10-4-2-3-5-10/h6-10H,2-5H2,1H

InchiKey: YKQPMEUETFVVNA-UHFFFAOYSA-N

Formula: C13H17NO2

SMILES: COc1ccc(NC(=O)C2CCCC2)cc1

Mol. weight [g/mol]: 219.28

Physical Properties

Property code	Value	Unit	Source
gf	53.38	kJ/mol	Joback Method
hf	-217.44	kJ/mol	Joback Method
hfus	24.90	kJ/mol	Joback Method
hvap	63.32	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.824		Crippen Method
mcvol	176.830	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
tb	670.24	K	Joback Method
tc	901.30	K	Joback Method
tf	410.93	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.92	J/mol×K	670.24	Joback Method
cpg	503.10	J/mol×K	708.75	Joback Method
cpg	519.04	J/mol×K	747.26	Joback Method
cpg	533.79	J/mol×K	785.77	Joback Method
cpg	547.40	J/mol×K	824.28	Joback Method
cpg	559.90	J/mol×K	862.79	Joback Method
cpg	571.34	J/mol×K	901.30	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307027&Units=SI

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