Cyclopropanecarboxamide, N-(4-methoxyphenyl)-

Inchi: InChI=1S/C11H13NO2/c1-14-10-6-4-9(5-7-10)12-11(13)8-2-3-8/h4-8H,2-3H2,1H3,(H,12,

InchiKey: SNPUKRLJGLDWRT-UHFFFAOYSA-N

Formula: C11H13NO2

SMILES: COc1ccc(NC(=O)C2CC2)cc1

Mol. weight [g/mol]: 191.23

Physical Properties

Property code	Value	Unit	Source
gf	60.74	kJ/mol	Joback Method
hf	-163.84	kJ/mol	Joback Method
hfus	23.92	kJ/mol	Joback Method
hvap	58.52	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.044		Crippen Method
mcvol	148.650	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	1831.00		NIST Webbook
tb	615.94	K	Joback Method
tc	840.97	K	Joback Method
tf	395.43	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.84	J/mol×K	615.94	Joback Method
cpg	395.35	J/mol×K	653.45	Joback Method
cpg	408.87	J/mol×K	690.95	Joback Method
cpg	421.45	J/mol×K	728.46	Joback Method
cpg	433.15	J/mol×K	765.96	Joback Method
cpg	444.01	J/mol×K	803.47	Joback Method
cpg	454.10	J/mol×K	840.97	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=U307188&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume