Cyclopentanecarboxamide, N-(2,5-dimethoxyphenyl)-

Inchi: InChI=1S/C14H19NO3/c1-17-11-7-8-13(18-2)12(9-11)15-14(16)10-5-3-4-6-10/h7-10H,3-

InchiKey: GMZSYRSBAMAPFL-UHFFFAOYSA-N

Formula: C14H19NO3

SMILES: COc1ccc(OC)c(NC(=O)C2CCCC2)c1

Mol. weight [g/mol]: 249.31

Physical Properties

Property code	Value	Unit	Source
gf	-52.83	kJ/mol	Joback Method
hf	-381.77	kJ/mol	Joback Method
hfus	28.29	kJ/mol	Joback Method
hvap	68.62	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.833		Crippen Method
mcvol	196.790	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	2131.00		NIST Webbook
rinpol	2131.00		NIST Webbook
tb	720.52	K	Joback Method
tc	945.21	K	Joback Method
tf	456.95	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.87	J/mol×K	720.52	Joback Method
cpg	582.68	J/mol×K	757.97	Joback Method
cpg	598.28	J/mol×K	795.42	Joback Method
cpg	612.71	J/mol×K	832.87	Joback Method
cpg	625.97	J/mol×K	870.31	Joback Method
cpg	638.09	J/mol×K	907.76	Joback Method
cpg	649.09	J/mol×K	945.21	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=U307029&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