Cyclopentanecarboxylic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C13H16O3/c1-15-11-6-8-12(9-7-11)16-13(14)10-4-2-3-5-10/h6-10H,2-5H2,1H3

InchiKey: ORMAVLLFHICVKM-UHFFFAOYSA-N

Formula: C13H16O3

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

Mol. weight [g/mol]: 220.26

Physical Properties

Property code	Value	Unit	Source
gf	-141.01	kJ/mol	Joback Method
hf	-403.13	kJ/mol	Joback Method
hfus	20.99	kJ/mol	Joback Method
hvap	59.29	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.791		Crippen Method
mcvol	172.720	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	1741.00		NIST Webbook
tb	642.49	K	Joback Method
tc	872.23	K	Joback Method
tf	380.50	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.45	J/mol×K	642.49	Joback Method
cpg	475.92	J/mol×K	680.78	Joback Method
cpg	492.20	J/mol×K	719.07	Joback Method
cpg	507.33	J/mol×K	757.36	Joback Method
cpg	521.33	J/mol×K	795.65	Joback Method
cpg	534.21	J/mol×K	833.94	Joback Method
cpg	546.01	J/mol×K	872.23	Joback Method
dvisc	0.0014553	Pa×s	380.50	Joback Method
dvisc	0.0008662	Pa×s	424.17	Joback Method

dvisc	0.0005679	Pa×s	467.83	Joback Method
dvisc	0.0004002	Pa×s	511.50	Joback Method
dvisc	0.0002980	Pa×s	555.16	Joback Method
dvisc	0.0002316	Pa×s	598.83	Joback Method
dvisc	0.0001863	Pa×s	642.49	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=U307577&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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