1-(4-Methoxyphenyl)-1-cyclopentanecarboxylic acid

Other names: Cyclopentanecarboxylic acid, 1-(4-methoxyphenyl)-
1-(4-Methoxyphenyl)cyclopentanecarboxylic acid
1-(4-methoxyphenyl)cyclopentane-1-carboxylic acid

Inchi: InChI=1S/C13H16O3/c1-16-11-6-4-10(5-7-11)13(12(14)15)8-2-3-9-13/h4-7H,2-3,8-9H2,1

InchiKey: OMMROWIAJMZSLF-UHFFFAOYSA-N

Formula: C13H16O3

SMILES: COc1ccc(C2(C(=O)O)CCCC2)cc1

Mol. weight [g/mol]: 220.26

CAS: 43050-28-8

Physical Properties

Property code	Value	Unit	Source
gf	-178.32	kJ/mol	Joback Method
hf	-407.90	kJ/mol	Joback Method
hfus	17.59	kJ/mol	Joback Method
hvap	72.41	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.592		Crippen Method
mcvol	172.720	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
tb	712.49	K	Joback Method
tc	934.91	K	Joback Method
tf	442.99	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.52	J/mol×K	712.49	Joback Method
cpg	499.82	J/mol×K	749.56	Joback Method
cpg	513.45	J/mol×K	786.63	Joback Method
cpg	526.53	J/mol×K	823.70	Joback Method
cpg	539.19	J/mol×K	860.77	Joback Method
cpg	551.56	J/mol×K	897.84	Joback Method

cpg	563.78	J/mol×K	934.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C43050288&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume