Cyclopentanecarboxylic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C14H18O2/c1-10-7-11(2)9-13(8-10)16-14(15)12-5-3-4-6-12/h7-9,12H,3-6H2,1-

InchiKey: OAWMOISULVJMCJ-UHFFFAOYSA-N

Formula: C14H18O2

SMILES: Cc1cc(C)cc(OC(=O)C2CCCC2)c1

Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
gf	-37.22	kJ/mol	Joback Method
hf	-303.02	kJ/mol	Joback Method
hfus	22.00	kJ/mol	Joback Method
hvap	59.77	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.399		Crippen Method
mcvol	180.940	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
rinpol	1679.00		NIST Webbook
tb	647.93	K	Joback Method
tc	877.34	K	Joback Method
tf	382.06	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.94	J/mol×K	647.93	Joback Method
cpg	501.10	J/mol×K	686.16	Joback Method
cpg	518.06	J/mol×K	724.40	Joback Method
cpg	533.84	J/mol×K	762.63	Joback Method
cpg	548.49	J/mol×K	800.87	Joback Method
cpg	562.04	J/mol×K	839.10	Joback Method
cpg	574.52	J/mol×K	877.34	Joback Method
dvisc	0.0015210	Pa×s	382.06	Joback Method
dvisc	0.0009224	Pa×s	426.37	Joback Method

dvisc	0.0006146	Pa×s	470.68	Joback Method
dvisc	0.0004391	Pa×s	515.00	Joback Method
dvisc	0.0003309	Pa×s	559.31	Joback Method
dvisc	0.0002600	Pa×s	603.62	Joback Method
dvisc	0.0002111	Pa×s	647.93	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=U307576&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