Cyclopentanecarboxylic acid, 3-methylphenyl ester

Inchi: InChI=1S/C13H16O2/c1-10-5-4-8-12(9-10)15-13(14)11-6-2-3-7-11/h4-5,8-9,11H,2-3,6-7H
InchiKey: LVDMYKFYZQJRAB-UHFFFAOYSA-N
Formula: C13H16O2
SMILES: Cc1cccc(OC(=O)C2CCCC2)c1
Mol. weight [g/mol]: 204.26

Physical Properties

Property code	Value	Unit	Source
gf	-36.01	kJ/mol	Joback Method
hf	-270.91	kJ/mol	Joback Method
hfus	19.80	kJ/mol	Joback Method
hvap	56.88	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.091		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1584.00		NIST Webbook
tb	620.07	K	Joback Method
tc	853.14	K	Joback Method
tf	358.27	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.75	J/mol×K	620.07	Joback Method
cpg	449.72	J/mol×K	658.92	Joback Method
cpg	466.46	J/mol×K	697.76	Joback Method
cpg	482.00	J/mol×K	736.61	Joback Method
cpg	496.40	J/mol×K	775.45	Joback Method
cpg	509.69	J/mol×K	814.30	Joback Method
cpg	521.92	J/mol×K	853.14	Joback Method
dvisc	0.0019305	Pa×s	358.27	Joback Method

dvisc	0.0011203	Pa×s	401.90	Joback Method
dvisc	0.0007232	Pa×s	445.54	Joback Method
dvisc	0.0005048	Pa×s	489.17	Joback Method
dvisc	0.0003737	Pa×s	532.80	Joback Method
dvisc	0.0002896	Pa×s	576.44	Joback Method
dvisc	0.0002326	Pa×s	620.07	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=U307574&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

Latest version available from:
https://www.chemeo.com/cid/61-957-2/Cyclopentanecarboxylic-acid-3-methylphenyl-ester.pdf
Generated by Cheméo on 2024-10-12 08:42:33.196709554 +0000 UTC m=+3303415.833678803.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.