Cyclopentanecarboxylic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C12H13ClO2/c13-10-5-7-11(8-6-10)15-12(14)9-3-1-2-4-9/h5-9H,1-4H2
InchiKey: ZMLQNIGUNYBKJO-UHFFFAOYSA-N
Formula: C12H13ClO2
SMILES: O=C(Oc1ccc(Cl)cc1)C1CCCC1
Mol. weight [g/mol]: 224.68

Physical Properties

Property code	Value	Unit	Source
gf	-56.36	kJ/mol	Joback Method
hf	-266.01	kJ/mol	Joback Method
hfus	21.41	kJ/mol	Joback Method
hvap	59.04	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.436		Crippen Method
mcvol	165.000	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	1663.00		NIST Webbook
tb	634.62	K	Joback Method
tc	875.78	K	Joback Method
tf	376.92	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.39	J/mol×K	634.62	Joback Method
cpg	425.57	J/mol×K	674.81	Joback Method
cpg	440.55	J/mol×K	715.01	Joback Method
cpg	454.35	J/mol×K	755.20	Joback Method
cpg	467.04	J/mol×K	795.39	Joback Method
cpg	478.65	J/mol×K	835.59	Joback Method
cpg	489.24	J/mol×K	875.78	Joback Method
dvisc	0.0018492	Pa×s	376.92	Joback Method
dvisc	0.0011123	Pa×s	419.87	Joback Method

dvisc	0.0007352	Pa×s	462.82	Joback Method
dvisc	0.0005214	Pa×s	505.77	Joback Method
dvisc	0.0003902	Pa×s	548.72	Joback Method
dvisc	0.0003046	Pa×s	591.67	Joback Method
dvisc	0.0002458	Pa×s	634.62	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=U307575&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

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