3-Cyclopentylpropionic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C14H17ClO2/c15-12-6-8-13(9-7-12)17-14(16)10-5-11-3-1-2-4-11/h6-9,11H,1-5

InchiKey: XVFXNEMYRISWTL-UHFFFAOYSA-N

Formula: C14H17ClO2

SMILES: O=C(CCC1CCCC1)Oc1ccc(Cl)cc1

Mol. weight [g/mol]: 252.74

Physical Properties

Property code	Value	Unit	Source
gf	-39.52	kJ/mol	Joback Method
hf	-307.29	kJ/mol	Joback Method
hfus	26.59	kJ/mol	Joback Method
hvap	63.49	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.216		Crippen Method
mcvol	193.180	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	1887.00		NIST Webbook
rinpol	1887.00		NIST Webbook
tb	680.38	K	Joback Method
tc	911.85	K	Joback Method
tf	399.46	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.30	J/mol×K	680.38	Joback Method
cpg	585.59	J/mol×K	873.27	Joback Method
cpg	573.22	J/mol×K	834.69	Joback Method
cpg	559.75	J/mol×K	796.11	Joback Method
cpg	545.15	J/mol×K	757.54	Joback Method
cpg	529.34	J/mol×K	718.96	Joback Method
cpg	596.91	J/mol×K	911.85	Joback Method
dvisc	0.0002009	Pa×s	680.38	Joback Method

dvisc	0.0002513	Pa×s	633.56	Joback Method
dvisc	0.0003257	Pa×s	586.74	Joback Method
dvisc	0.0004417	Pa×s	539.92	Joback Method
dvisc	0.0006348	Pa×s	493.10	Joback Method
dvisc	0.0009842	Pa×s	446.28	Joback Method
dvisc	0.0016912	Pa×s	399.46	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=U307131&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