

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
rinsol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.39	J/molxK	634.62	Joback Method
cpg	478.65	J/molxK	835.59	Joback Method
cpg	467.04	J/molxK	795.39	Joback Method
cpg	454.35	J/molxK	755.20	Joback Method
cpg	440.55	J/molxK	715.01	Joback Method
cpg	425.57	J/molxK	674.81	Joback Method
cpg	489.24	J/molxK	875.78	Joback Method
dvisc	0.0002458	Paxs	634.62	Joback Method
dvisc	0.0003046	Paxs	591.67	Joback Method

dvisc	0.0003902	Paxs	548.72	Joback Method
dvisc	0.0005214	Paxs	505.77	Joback Method
dvisc	0.0007352	Paxs	462.82	Joback Method
dvisc	0.0011123	Paxs	419.87	Joback Method
dvisc	0.0018492	Paxs	376.92	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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