

2-Methylpropionic acid, 4-chlorophenyl ester

Inchi:	InChI=1S/C10H11ClO2/c1-7(2)10(12)13-9-5-3-8(11)4-6-9/h3-7H,1-2H3
InchiKey:	WPCAYDFRIDVTNI-UHFFFAOYSA-N
Formula:	C10H11ClO2
SMILES:	CC(C)C(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	198.65

Physical Properties

Property code	Value	Unit	Source
gf	-112.19	kJ/mol	Joback Method
hf	-290.49	kJ/mol	Joback Method
hfus	18.77	kJ/mol	Joback Method
hvap	53.95	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.901		Crippen Method
mcvol	147.680	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinsol	1356.00		NIST Webbook
tb	573.14	K	Joback Method
tc	796.07	K	Joback Method
tf	328.48	K	Joback Method
vc	0.554	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.36	J/molxK	573.14	Joback Method
cpg	339.19	J/molxK	610.30	Joback Method
cpg	351.23	J/molxK	647.45	Joback Method
cpg	362.51	J/molxK	684.61	Joback Method
cpg	373.05	J/molxK	721.76	Joback Method
cpg	382.87	J/molxK	758.92	Joback Method
cpg	391.97	J/molxK	796.07	Joback Method
dvisc	0.0020698	Paxs	328.48	Joback Method
dvisc	0.0011257	Paxs	369.26	Joback Method

dvisc	0.0006911	Paxs	410.03	Joback Method
dvisc	0.0004634	Paxs	450.81	Joback Method
dvisc	0.0003321	Paxs	491.59	Joback Method
dvisc	0.0002504	Paxs	532.36	Joback Method
dvisc	0.0001966	Paxs	573.14	Joback Method

Sources

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=U308015&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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