4-Chlorophenyl-«beta»-phenylpropionate

Other names: 4-Chlorophenyl 3-phenylpropanoate
3-Phenylpropionic acid, 4-chlorophenyl ester
Inchi: InChI=1S/C15H13ClO2/c16-13-7-9-14(10-8-13)18-15(17)11-6-12-4-2-1-3-5-12/h1-5,7-10
InchiKey: KYCIZZNPNUORSI-UHFFFAOYSA-N
Formula: C15H13ClO2
SMILES: O=C(CCc1ccccc1)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 260.72
CAS: 23522-73-8

Physical Properties

Property code	Value	Unit	Source
gf	44.76	kJ/mol	Joback Method
hf	-151.88	kJ/mol	Joback Method
hfus	29.28	kJ/mol	Joback Method
hvap	67.74	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.878		Crippen Method
mcvol	194.370	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1996.00		NIST Webbook
tb	714.66	K	Joback Method
tc	955.69	K	Joback Method
tf	426.25	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.15	J/mol×K	714.66	Joback Method
cpg	505.40	J/mol×K	754.83	Joback Method
cpg	518.48	J/mol×K	795.00	Joback Method
cpg	530.44	J/mol×K	835.17	Joback Method
cpg	541.33	J/mol×K	875.35	Joback Method
cpg	551.20	J/mol×K	915.52	Joback Method

cpg	560.11	J/mol×K	955.69	Joback Method
dvisc	0.0010871	Pa×s	426.25	Joback Method
dvisc	0.0006325	Pa×s	474.32	Joback Method
dvisc	0.0004066	Pa×s	522.39	Joback Method
dvisc	0.0002815	Pa×s	570.45	Joback Method
dvisc	0.0002064	Pa×s	618.52	Joback Method
dvisc	0.0001583	Pa×s	666.59	Joback Method
dvisc	0.0001258	Pa×s	714.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23522738&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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