5-Phenylvaleric acid, 4-chlorophenyl ester

Inchi: InChI=1S/C17H17ClO2/c18-15-10-12-16(13-11-15)20-17(19)9-5-4-8-14-6-2-1-3-7-14/h1-
InchiKey: QTDNOYVRUFYGHX-UHFFFAOYSA-N
Formula: C17H17ClO2
SMILES: O=C(CCCCc1ccccc1)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 288.77

Physical Properties

Property code	Value	Unit	Source
gf	61.60	kJ/mol	Joback Method
hf	-193.16	kJ/mol	Joback Method
hfus	34.46	kJ/mol	Joback Method
hvap	72.19	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.658		Crippen Method
mcvol	222.550	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpol	2272.00		NIST Webbook
rinpol	2272.00		NIST Webbook
tb	760.42	K	Joback Method
tc	992.42	K	Joback Method
tf	448.79	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.51	J/mol×K	760.42	Joback Method
cpg	612.43	J/mol×K	799.09	Joback Method
cpg	626.16	J/mol×K	837.75	Joback Method
cpg	638.76	J/mol×K	876.42	Joback Method
cpg	650.28	J/mol×K	915.09	Joback Method
cpg	660.78	J/mol×K	953.76	Joback Method
cpg	670.31	J/mol×K	992.42	Joback Method
dvisc	0.0009408	Pa×s	448.79	Joback Method

dvisc	0.0005320	Pa×s	500.73	Joback Method
dvisc	0.0003349	Pa×s	552.67	Joback Method
dvisc	0.0002282	Pa×s	604.61	Joback Method
dvisc	0.0001653	Pa×s	656.54	Joback Method
dvisc	0.0001255	Pa×s	708.48	Joback Method
dvisc	0.0000989	Pa×s	760.42	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=U406900&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