Phenylacetic acid, 4-chloro-, propyl ester

Inchi: InChI=1S/C11H13ClO2/c1-2-7-14-11(13)8-9-3-5-10(12)6-4-9/h3-6H,2,7-8H2,1H3
InchiKey: OKKOZFNOMZSZBQ-UHFFFAOYSA-N
Formula: C11H13ClO2
SMILES: CCCOC(=O)Cc1ccc(Cl)cc1
Mol. weight [g/mol]: 212.67

Physical Properties

Property code	Value	Unit	Source
gf	-101.33	kJ/mol	Joback Method
hf	-305.85	kJ/mol	Joback Method
hfus	24.88	kJ/mol	Joback Method
hvap	56.56	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.836		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	1546.00		NIST Webbook
tb	596.46	K	Joback Method
tc	810.87	K	Joback Method
tf	354.75	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.82	J/mol×K	596.46	Joback Method
cpg	386.14	J/mol×K	632.19	Joback Method
cpg	398.67	J/mol×K	667.93	Joback Method
cpg	410.44	J/mol×K	703.66	Joback Method
cpg	421.46	J/mol×K	739.40	Joback Method
cpg	431.76	J/mol×K	775.13	Joback Method
cpg	441.35	J/mol×K	810.87	Joback Method
dvisc	0.0016178	Pa×s	354.75	Joback Method
dvisc	0.0009457	Pa×s	395.04	Joback Method

dvisc	0.0006105	Pa×s	435.32	Joback Method
dvisc	0.0004245	Pa×s	475.61	Joback Method
dvisc	0.0003124	Pa×s	515.89	Joback Method
dvisc	0.0002403	Pa×s	556.17	Joback Method
dvisc	0.0001915	Pa×s	596.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406207&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