Phenylacetic acid, 4-chloro-, pentyl ester

Inchi: InChI=1S/C13H17ClO2/c1-2-3-4-9-16-13(15)10-11-5-7-12(14)8-6-11/h5-8H,2-4,9-10H2,1
InchiKey: YKZPKZQCLCQSSB-UHFFFAOYSA-N
Formula: C13H17ClO2
SMILES: CCCCCOC(=O)Cc1ccc(Cl)cc1
Mol. weight [g/mol]: 240.73

Physical Properties

Property code	Value	Unit	Source
gf	-84.49	kJ/mol	Joback Method
hf	-347.13	kJ/mol	Joback Method
hfus	30.06	kJ/mol	Joback Method
hvap	61.01	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.616		Crippen Method
mcvol	189.950	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1742.00		NIST Webbook
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tb	642.22	K	Joback Method
tc	849.84	K	Joback Method
tf	377.29	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.36	J/mol×K	642.22	Joback Method
cpg	536.14	J/mol×K	815.23	Joback Method
cpg	524.81	J/mol×K	780.63	Joback Method
cpg	512.68	J/mol×K	746.03	Joback Method
cpg	499.75	J/mol×K	711.43	Joback Method
cpg	485.98	J/mol×K	676.82	Joback Method
cpg	546.71	J/mol×K	849.84	Joback Method
dvisc	0.0001562	Pa×s	642.22	Joback Method

dvisc	0.0001978	Pa×s	598.07	Joback Method
dvisc	0.0002602	Pa×s	553.91	Joback Method
dvisc	0.0003589	Pa×s	509.75	Joback Method
dvisc	0.0005262	Pa×s	465.60	Joback Method
dvisc	0.0008357	Pa×s	421.45	Joback Method
dvisc	0.0014793	Pa×s	377.29	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=U406209&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