Phenylacetic acid, 4-chloro-, heptyl ester

Inchi: InChI=1S/C15H21ClO2/c1-2-3-4-5-6-11-18-15(17)12-13-7-9-14(16)10-8-13/h7-10H,2-6,1
InchiKey: PASLQPGQXAOSNK-UHFFFAOYSA-N
Formula: C15H21ClO2
SMILES: CCCCCCCOC(=O)Cc1ccc(Cl)cc1
Mol. weight [g/mol]: 268.78

Physical Properties

Property code	Value	Unit	Source
gf	-67.65	kJ/mol	Joback Method
hf	-388.41	kJ/mol	Joback Method
hfus	35.24	kJ/mol	Joback Method
hvap	65.46	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.396		Crippen Method
mcvol	218.130	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
rinpol	1943.00		NIST Webbook
rinpol	1943.00		NIST Webbook
tb	687.98	K	Joback Method
tc	890.06	K	Joback Method
tf	399.83	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.67	J/mol×K	687.98	Joback Method
cpg	591.24	J/mol×K	721.66	Joback Method
cpg	605.90	J/mol×K	755.34	Joback Method
cpg	619.68	J/mol×K	789.02	Joback Method
cpg	632.59	J/mol×K	822.70	Joback Method
cpg	644.67	J/mol×K	856.38	Joback Method
cpg	655.94	J/mol×K	890.06	Joback Method
dvisc	0.0013068	Pa×s	399.83	Joback Method

dvisc	0.0007157	Pa×s	447.86	Joback Method
dvisc	0.0004405	Pa×s	495.88	Joback Method
dvisc	0.0002954	Pa×s	543.90	Joback Method
dvisc	0.0002113	Pa×s	591.93	Joback Method
dvisc	0.0001590	Pa×s	639.96	Joback Method
dvisc	0.0001245	Pa×s	687.98	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406211&Units=SI

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