Phenylacetic acid, 3-chloroprop-2-enyl ester

Inchi: InChI=1S/C11H11ClO2/c12-7-4-8-14-11(13)9-10-5-2-1-3-6-10/h1-7H,8-9H2/b7-4+
InchiKey: PBULRLQIJUOCDV-QPJJXVBHSA-N
Formula: C11H11ClO2
SMILES: O=C(Cc1ccccc1)OCC=CCl
Mol. weight [g/mol]: 210.66

Physical Properties

Property code	Value	Unit	Source
gf	-11.48	kJ/mol	Joback Method
hf	-177.16	kJ/mol	Joback Method
hfus	25.47	kJ/mol	Joback Method
hvap	55.86	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.525		Crippen Method
mcvol	157.470	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
rinpol	1563.20		NIST Webbook
tb	595.64	K	Joback Method
tc	818.39	K	Joback Method
tf	337.15	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.13	J/mol×K	595.64	Joback Method
cpg	409.48	J/mol×K	781.26	Joback Method
cpg	399.80	J/mol×K	744.14	Joback Method
cpg	389.37	J/mol×K	707.01	Joback Method
cpg	378.14	J/mol×K	669.89	Joback Method
cpg	366.08	J/mol×K	632.76	Joback Method
cpg	418.45	J/mol×K	818.39	Joback Method
dvisc	0.0001667	Pa×s	595.64	Joback Method
dvisc	0.0002136	Pa×s	552.56	Joback Method

dvisc	0.0002855	Pa×s	509.48	Joback Method
dvisc	0.0004026	Pa×s	466.39	Joback Method
dvisc	0.0006088	Pa×s	423.31	Joback Method
dvisc	0.0010111	Pa×s	380.23	Joback Method
dvisc	0.0019117	Pa×s	337.15	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=U292539&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