Phenylacetic acid, 3-chloro, methyl ester

Inchi: InChI=1S/C9H9ClO2/c1-12-9(11)6-7-3-2-4-8(10)5-7/h2-5H,6H2,1H3
InchiKey: HTBBVKFFDDQVER-UHFFFAOYSA-N
Formula: C9H9ClO2
SMILES: COC(=O)Cc1cccc(Cl)c1
Mol. weight [g/mol]: 184.62

Physical Properties

Property code	Value	Unit	Source
gf	-118.17	kJ/mol	Joback Method
hf	-264.57	kJ/mol	Joback Method
hfus	19.70	kJ/mol	Joback Method
hvap	52.11	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.055		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
rinpol	1304.30		NIST Webbook
rinpol	1340.50		NIST Webbook
rinpol	1304.30		NIST Webbook
tb	550.70	K	Joback Method
tc	772.80	K	Joback Method
tf	332.21	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.82	J/mol×K	550.70	Joback Method
cpg	331.82	J/mol×K	735.78	Joback Method
cpg	322.92	J/mol×K	698.76	Joback Method
cpg	313.39	J/mol×K	661.75	Joback Method
cpg	303.20	J/mol×K	624.73	Joback Method
cpg	292.35	J/mol×K	587.72	Joback Method
cpg	340.09	J/mol×K	772.80	Joback Method

dvisc	0.0002281	Pa×s	550.70	Joback Method
dvisc	0.0002831	Pa×s	514.29	Joback Method
dvisc	0.0003631	Pa×s	477.87	Joback Method
dvisc	0.0004852	Pa×s	441.46	Joback Method
dvisc	0.0006831	Pa×s	405.04	Joback Method
dvisc	0.0010290	Pa×s	368.63	Joback Method
dvisc	0.0016956	Pa×s	332.21	Joback Method

Sources

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=R216741&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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