

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/molxK	550.70	Joback Method
cpg	331.82	J/molxK	735.78	Joback Method
cpg	322.92	J/molxK	698.76	Joback Method
cpg	313.39	J/molxK	661.75	Joback Method
cpg	303.20	J/molxK	624.73	Joback Method
cpg	292.35	J/molxK	587.72	Joback Method
cpg	340.09	J/molxK	772.80	Joback Method

dvisc	0.0002281	Paxs	550.70	Joback Method
dvisc	0.0002831	Paxs	514.29	Joback Method
dvisc	0.0003631	Paxs	477.87	Joback Method
dvisc	0.0004852	Paxs	441.46	Joback Method
dvisc	0.0006831	Paxs	405.04	Joback Method
dvisc	0.0010290	Paxs	368.63	Joback Method
dvisc	0.0016956	Paxs	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/ci9903071
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
mvol:	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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