

Methyl «alpha»-chlorophenylacetate

Other names:	Methyl chloro(phenyl)acetate Methyl alpha-chlorophenylacetate Methyl a-chlorophenylacetate
Inchi:	InChI=1S/C9H9ClO2/c1-12-9(11)8(10)7-5-3-2-4-6-7/h2-6,8H,1H3
InchiKey:	XOIOYHPJZJLTGK-UHFFFAOYSA-N
Formula:	C9H9ClO2
SMILES:	COC(=O)C(Cl)c1ccccc1
Mol. weight [g/mol]:	184.62
CAS:	7476-66-6

Physical Properties

Property code	Value	Unit	Source
gf	-110.98	kJ/mol	Joback Method
hf	-258.38	kJ/mol	Joback Method
hfus	16.57	kJ/mol	Joback Method
hvap	51.06	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	2.139		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
tb	545.28	K	Joback Method
tc	771.28	K	Joback Method
tf	304.69	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.82	J/molxK	545.28	Joback Method
cpg	335.15	J/molxK	733.61	Joback Method
cpg	325.96	J/molxK	695.95	Joback Method
cpg	316.05	J/molxK	658.28	Joback Method
cpg	305.41	J/molxK	620.61	Joback Method
cpg	294.01	J/molxK	582.95	Joback Method

cpg	343.63	J/molxK	771.28	Joback Method
dvisc	0.0002204	Paxs	545.28	Joback Method
dvisc	0.0002851	Paxs	505.18	Joback Method
dvisc	0.0003856	Paxs	465.08	Joback Method
dvisc	0.0005521	Paxs	424.99	Joback Method
dvisc	0.0008517	Paxs	384.89	Joback Method
dvisc	0.0014534	Paxs	344.79	Joback Method
dvisc	0.0028549	Paxs	304.69	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	402.50 ± 1.50	K	2.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C7476666&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
tb:	Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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