Methyl 4-chloro-3-methylbenzoate

Other names: Benzoic acid, 4-chloro-3-methyl-, methyl ester
Inchi: InChI=1S/C9H9ClO2/c1-6-5-7(9(11)12-2)3-4-8(6)10/h3-5H,1-2H3
InchiKey: QOTGNXMPQNGYDM-UHFFFAOYSA-N
Formula: C9H9ClO2
SMILES: COC(=O)c1ccc(Cl)c(C)c1
Mol. weight [g/mol]: 184.62
CAS: 91367-05-4

Physical Properties

Property code	Value	Unit	Source
gf	-127.80	kJ/mol	Joback Method
hf	-276.04	kJ/mol	Joback Method
hfus	19.31	kJ/mol	Joback Method
hvap	52.77	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.435		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
tb	555.68	K	Joback Method
tc	778.87	K	Joback Method
tf	344.73	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.08	J/mol×K	555.68	Joback Method
cpg	291.31	J/mol×K	592.88	Joback Method
cpg	301.92	J/mol×K	630.08	Joback Method
cpg	311.91	J/mol×K	667.27	Joback Method
cpg	321.30	J/mol×K	704.47	Joback Method
cpg	330.08	J/mol×K	741.67	Joback Method
cpg	338.26	J/mol×K	778.87	Joback Method
dvisc	0.0013360	Pa×s	344.73	Joback Method

dvisc	0.0008629	Pa×s	379.89	Joback Method
dvisc	0.0006002	Pa×s	415.05	Joback Method
dvisc	0.0004418	Pa×s	450.20	Joback Method
dvisc	0.0003399	Pa×s	485.36	Joback Method
dvisc	0.0002710	Pa×s	520.52	Joback Method
dvisc	0.0002223	Pa×s	555.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91367054&Units=SI
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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume