Methyl 3-chloro-4-methoxybenzoate

Other names: Benzoic acid, 3-chloro-4-methoxy-, methyl ester
3-Cl-4-CH3O-C6H3-COOCH3
methyl 3-chloro-p-anisate
Inchi: InChI=1S/C9H9ClO3/c1-12-8-4-3-6(5-7(8)10)9(11)13-2/h3-5H,1-2H3
InchiKey: PINQDVFQCCFACD-UHFFFAOYSA-N
Formula: C9H9ClO3
SMILES: COC(=O)c1ccc(OC)c(Cl)c1
Mol. weight [g/mol]: 200.62
CAS: 37908-98-8

Physical Properties

Property code	Value	Unit	Source
affp	858.40	kJ/mol	NIST Webbook
basg	827.50	kJ/mol	NIST Webbook
gf	-232.80	kJ/mol	Joback Method
hf	-408.26	kJ/mol	Joback Method
hfus	20.50	kJ/mol	Joback Method
hvap	55.18	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.135		Crippen Method
mcvol	139.460	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
tb	578.10	K	Joback Method
tc	798.52	K	Joback Method
tf	366.96	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.40	J/mol×K	578.10	Joback Method
cpg	313.52	J/mol×K	614.84	Joback Method
cpg	324.06	J/mol×K	651.57	Joback Method
cpg	334.01	J/mol×K	688.31	Joback Method

cpg	343.37	J/mol×K	725.05	Joback Method
cpg	352.12	J/mol×K	761.78	Joback Method
cpg	360.25	J/mol×K	798.52	Joback Method
dvisc	0.0010339	Pa×s	366.96	Joback Method
dvisc	0.0006811	Pa×s	402.15	Joback Method
dvisc	0.0004798	Pa×s	437.34	Joback Method
dvisc	0.0003562	Pa×s	472.53	Joback Method
dvisc	0.0002755	Pa×s	507.72	Joback Method
dvisc	0.0002203	Pa×s	542.91	Joback Method
dvisc	0.0001811	Pa×s	578.10	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37908988&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

affp: Proton affinity
basg: Gas basicity
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