4-Chlorobenzoic acid, 4-methoxyphenyl ester

Other names: 4-Chlorobenzoic acid, 4-methoxyphenyl ester
4-Methoxyphenyl 4-chlorobenzoate
Benzoic acid, 4-chloro-, 4-methoxyphenyl ester
Inchi: InChI=1S/C14H11ClO3/c1-17-12-6-8-13(9-7-12)18-14(16)10-2-4-11(15)5-3-10/h2-9H,1H
InchiKey: MSZPFWFDFWYVOE-UHFFFAOYSA-N
Formula: C14H11ClO3
SMILES: COc1ccc(OC(=O)c2ccc(Cl)cc2)cc1
Mol. weight [g/mol]: 262.69

Physical Properties

Property code	Value	Unit	Source
hf	-332.31	kJ/mol	Cheméo Relay (1.0)
hfus	27.49	kJ/mol	Joback Method
hvap	93.24	kJ/mol	Cheméo Relay (1.0)
ie	8.12	eV	Cheméo Relay (1.0)
log10ws	-4.81		Cheméo Relay (1.0)
logp	3.568		Crippen Method
mcvol	186.150	ml/mol	McGowan Method
rinpol	2074.00		NIST Webbook
rinpol	2074.00		NIST Webbook
tb	631.14	K	Cheméo Relay (1.0)
tf	354.32	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.12	J/mol×K	719.18	Joback Method
cpg	476.37	J/mol×K	759.70	Joback Method
cpg	488.52	J/mol×K	800.21	Joback Method
cpg	499.56	J/mol×K	840.73	Joback Method
cpg	509.54	J/mol×K	881.24	Joback Method
cpg	518.46	J/mol×K	921.76	Joback Method
cpg	526.34	J/mol×K	962.28	Joback Method
dvisc	0.0007169	Pa×s	449.73	Joback Method

dvisc	0.0004548	Pa×s	494.64	Joback Method
dvisc	0.0003112	Pa×s	539.55	Joback Method
dvisc	0.0002257	Pa×s	584.45	Joback Method
dvisc	0.0001714	Pa×s	629.36	Joback Method
dvisc	0.0001350	Pa×s	674.27	Joback Method
dvisc	0.0001096	Pa×s	719.18	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5410991&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point