o-Anisic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C14H11ClO3/c1-17-13-5-3-2-4-12(13)14(16)18-11-8-6-10(15)7-9-11/h2-9H,1H
InchiKey: BELPBVCDOMAVAK-UHFFFAOYSA-N
Formula: C14H11ClO3
SMILES: COc1ccccc1C(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 262.69

Physical Properties

Property code	Value	Unit	Source
gf	-78.29	kJ/mol	Joback Method
hf	-274.93	kJ/mol	Joback Method
hfus	27.49	kJ/mol	Joback Method
hvap	68.58	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.568		Crippen Method
mcvol	186.150	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpol	2046.00		NIST Webbook
rinpol	2046.00		NIST Webbook
tb	719.18	K	Joback Method
tc	962.28	K	Joback Method
tf	449.73	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.12	J/mol×K	719.18	Joback Method
cpg	518.46	J/mol×K	921.76	Joback Method
cpg	509.54	J/mol×K	881.24	Joback Method
cpg	499.56	J/mol×K	840.73	Joback Method
cpg	488.52	J/mol×K	800.21	Joback Method
cpg	476.37	J/mol×K	759.70	Joback Method
cpg	526.34	J/mol×K	962.28	Joback Method
dvisc	0.0001096	Pa×s	719.18	Joback Method

dvisc	0.0001350	Pa×s	674.27	Joback Method
dvisc	0.0001714	Pa×s	629.36	Joback Method
dvisc	0.0002257	Pa×s	584.45	Joback Method
dvisc	0.0003112	Pa×s	539.55	Joback Method
dvisc	0.0004548	Pa×s	494.64	Joback Method
dvisc	0.0007169	Pa×s	449.73	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=U307790&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
mcvol:	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