m-Anisic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C14H10Cl2O3/c1-18-10-4-2-3-9(7-10)14(17)19-11-5-6-12(15)13(16)8-11/h2-8H
InchiKey: NKZQQSMRSOXSET-UHFFFAOYSA-N
Formula: C14H10Cl2O3
SMILES: COc1cccc(C(=O)Oc2ccc(Cl)c(Cl)c2)c1
Mol. weight [g/mol]: 297.13

Physical Properties

Property code	Value	Unit	Source
gf	-99.85	kJ/mol	Joback Method
hf	-302.14	kJ/mol	Joback Method
hfus	31.30	kJ/mol	Joback Method
hvap	73.63	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.221		Crippen Method
mcvol	198.390	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	2262.00		NIST Webbook
rinpol	2262.00		NIST Webbook
tb	761.59	K	Joback Method
tc	1007.60	K	Joback Method
tf	492.17	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.05	J/mol×K	761.59	Joback Method
cpg	495.91	J/mol×K	802.59	Joback Method
cpg	506.68	J/mol×K	843.59	Joback Method
cpg	516.38	J/mol×K	884.59	Joback Method
cpg	525.01	J/mol×K	925.60	Joback Method
cpg	532.59	J/mol×K	966.60	Joback Method
cpg	539.12	J/mol×K	1007.60	Joback Method
dvisc	0.0005499	Pa×s	492.17	Joback Method

dvisc	0.0003674	Pa×s	537.07	Joback Method
dvisc	0.0002612	Pa×s	581.98	Joback Method
dvisc	0.0001950	Pa×s	626.88	Joback Method
dvisc	0.0001514	Pa×s	671.78	Joback Method
dvisc	0.0001213	Pa×s	716.69	Joback Method
dvisc	0.0000998	Pa×s	761.59	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307803&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume