P-anisic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C14H10Cl2O3/c1-18-10-4-2-9(3-5-10)14(17)19-11-6-7-12(15)13(16)8-11/h2-8H
InchiKey: FRVXSRVZQSAALV-UHFFFAOYSA-N
Formula: C14H10Cl2O3
SMILES: COc1ccc(C(=O)Oc2ccc(Cl)c(Cl)c2)cc1
Mol. weight [g/mol]: 297.14

Physical Properties

Property code	Value	Unit	Source
hf	-366.31	kJ/mol	Cheméo Relay (1.0)
hfus	31.30	kJ/mol	Joback Method
hvap	99.57	kJ/mol	Cheméo Relay (1.0)
ie	8.23	eV	Cheméo Relay (1.0)
log10ws	-5.64		Cheméo Relay (1.0)
logp	4.221		Crippen Method
mcvol	198.390	ml/mol	McGowan Method
rinpol	2323.00		NIST Webbook
tb	633.35	K	Cheméo Relay (1.0)
tf	355.17	K	Cheméo Relay (1.0)

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

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
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=U307638&Units=SI

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