

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/h2-8
InchiKey:	FRVXSRVZQSAALV-UHFFFAOYSA-N
Formula:	C14H10Cl2O3
SMILES:	COc1ccc(C(=O)Oc2ccc(Cl)c(Cl)c2)cc1
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
rinsol	2323.00		NIST Webbook
tb	761.59	K	Joback Method
tc	1007.60	K	Joback Method
tf	492.17	K	Joback Method
vc	0.744	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.05	J/molxK	761.59	Joback Method
cpg	495.91	J/molxK	802.59	Joback Method
cpg	506.68	J/molxK	843.59	Joback Method
cpg	516.38	J/molxK	884.59	Joback Method
cpg	525.01	J/molxK	925.60	Joback Method
cpg	532.59	J/molxK	966.60	Joback Method
cpg	539.12	J/molxK	1007.60	Joback Method
dvisc	0.0005499	Paxs	492.17	Joback Method
dvisc	0.0003674	Paxs	537.07	Joback Method

dvisc	0.0002612	Paxs	581.98	Joback Method
dvisc	0.0001950	Paxs	626.88	Joback Method
dvisc	0.0001514	Paxs	671.78	Joback Method
dvisc	0.0001213	Paxs	716.69	Joback Method
dvisc	0.0000998	Paxs	761.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307638&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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