

m-Anisic acid, 4-chlorophenyl ester

Inchi:	InChI=1S/C14H11ClO3/c1-17-13-4-2-3-10(9-13)14(16)18-12-7-5-11(15)6-8-12/h2-9H,1H
InchiKey:	NSYNJRZBHCVYKP-UHFFFAOYSA-N
Formula:	C14H11ClO3
SMILES:	COc1cccc(C(=O)Oc2ccc(Cl)cc2)c1
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
rinsol	2066.00		NIST Webbook
tb	719.18	K	Joback Method
tc	962.28	K	Joback Method
tf	449.73	K	Joback Method
vc	0.695	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.12	J/molxK	719.18	Joback Method
cpg	476.37	J/molxK	759.70	Joback Method
cpg	488.52	J/molxK	800.21	Joback Method
cpg	499.56	J/molxK	840.73	Joback Method
cpg	509.54	J/molxK	881.24	Joback Method
cpg	518.46	J/molxK	921.76	Joback Method
cpg	526.34	J/molxK	962.28	Joback Method
dvisc	0.0007169	Paxs	449.73	Joback Method
dvisc	0.0004548	Paxs	494.64	Joback Method

dvisc	0.0003112	Paxs	539.55	Joback Method
dvisc	0.0002257	Paxs	584.45	Joback Method
dvisc	0.0001714	Paxs	629.36	Joback Method
dvisc	0.0001350	Paxs	674.27	Joback Method
dvisc	0.0001096	Paxs	719.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307799&Units=SI
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

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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