p-Anisic anhydride

Other names:	4-Anisic anhydride
	4-Methoxybenzoic anhydride
	Benzoic acid, 4-methoxy-, anhydride
	p-Anisic acid anhydride
	p-Anisic anhydride
	p-Methoxybenzoic anhydride
Inchi:	InChI=1S/C16H14O5/c1-19-13-7-3-11(4-8-13)15(17)21-16(18)12-5-9-14(20-2)10-6-12/h3
InchiKey:	YGMHIBLUWGDWKP-UHFFFAOYSA-N
Formula:	C16H14O5
SMILES:	COc1ccc(C(=O)OC(=O)c2ccc(OC)cc2)cc1
Mol. weight [g/mol]:	286.28

Physical Properties

Property code	Value	Unit	Source
af	0.8281		Cheméo Relay (1.0)
hf	-628.67	kJ/mol	Cheméo Relay (1.0)
hfus	31.26	kJ/mol	Joback Method
hvap	99.81	kJ/mol	Cheméo Relay (1.0)
ie	8.22	eV	Cheméo Relay (1.0)
log10ws	-4.11		Cheméo Relay (1.0)
logp	2.701		Crippen Method
mcvol	209.530	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
tb	653.37	K	Cheméo Relay (1.0)
tc	898.53	K	Cheméo Relay (1.0)
tf	379.09	K	Cheméo Relay (1.0)
vc	0.776	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.87	J/mol×K	803.80	Joback Method
cpg	641.59	J/mol×K	1037.51	Joback Method
cpg	634.92	J/mol×K	998.56	Joback Method

cpg	627.00	J/mol×K	959.61	Joback Method
cpg	617.83	J/mol×K	920.65	Joback Method
cpg	607.42	J/mol×K	881.70	Joback Method
cpg	595.77	J/mol×K	842.75	Joback Method
dvisc	0.0001501	Pa×s	659.15	Joback Method
dvisc	0.0000730	Pa×s	803.80	Joback Method
dvisc	0.0000901	Pa×s	755.59	Joback Method
dvisc	0.0001143	Pa×s	707.37	Joback Method
dvisc	0.0004629	Pa×s	514.51	Joback Method
dvisc	0.0002060	Pa×s	610.94	Joback Method
dvisc	0.0002982	Pa×s	562.73	Joback Method

Sources

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=C794945&Units=SI
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

Legend

af:	Acentric Factor
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume