p-Anisic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C16H22O3/c1-4-5-6-7-8-13(2)19-16(17)14-9-11-15(18-3)12-10-14/h7-13H,4-6
InchiKey: NWEOELGGVACLOI-BQYQJAHWSA-N
Formula: C16H22O3
SMILES: CCCCC=CC(C)OC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 262.34

Physical Properties

Property code	Value	Unit	Source
gf	-74.52	kJ/mol	Joback Method
hf	-413.59	kJ/mol	Joback Method
hfus	31.50	kJ/mol	Joback Method
hvap	65.28	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	3.987		Crippen Method
mcvol	221.550	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	1946.00		NIST Webbook
rinpol	1946.00		NIST Webbook
tb	699.57	K	Joback Method
tc	904.52	K	Joback Method
tf	383.33	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.00	J/mol×K	699.57	Joback Method
cpg	678.75	J/mol×K	870.36	Joback Method
cpg	666.05	J/mol×K	836.20	Joback Method
cpg	652.45	J/mol×K	802.04	Joback Method
cpg	637.93	J/mol×K	767.89	Joback Method
cpg	622.45	J/mol×K	733.73	Joback Method
cpg	690.57	J/mol×K	904.52	Joback Method
dvisc	0.0000751	Pa×s	699.57	Joback Method

dvisc	0.0000982	Pa×s	646.86	Joback Method
dvisc	0.0001347	Pa×s	594.16	Joback Method
dvisc	0.0001965	Pa×s	541.45	Joback Method
dvisc	0.0003109	Pa×s	488.74	Joback Method
dvisc	0.0005496	Pa×s	436.04	Joback Method
dvisc	0.0011364	Pa×s	383.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299195&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