m-anisic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C16H22O3/c1-4-5-6-7-9-13(2)19-16(17)14-10-8-11-15(12-14)18-3/h7-13H,4-6
InchiKey: ILFVQCDACZZNIV-VQHVLOKHSA-N
Formula: C16H22O3
SMILES: CCCC/C=C/C(C)OC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 262.35

Physical Properties

Property code	Value	Unit	Source
hf	-481.37	kJ/mol	Cheméo Relay (1.0)
hfus	31.50	kJ/mol	Joback Method
hvap	85.61	kJ/mol	Cheméo Relay (1.0)
ie	8.36	eV	Cheméo Relay (1.0)
logp	3.987		Crippen Method
mcvol	221.550	ml/mol	McGowan Method
rinpol	1932.80		NIST Webbook
rinpol	1932.80		NIST Webbook
tb	581.53	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.00	J/mol×K	699.57	Joback Method
cpg	622.45	J/mol×K	733.73	Joback Method
cpg	637.93	J/mol×K	767.89	Joback Method
cpg	652.45	J/mol×K	802.04	Joback Method
cpg	666.05	J/mol×K	836.20	Joback Method
cpg	678.75	J/mol×K	870.36	Joback Method
cpg	690.57	J/mol×K	904.52	Joback Method
dvisc	0.0011364	Pa×s	383.33	Joback Method
dvisc	0.0005496	Pa×s	436.04	Joback Method
dvisc	0.0003109	Pa×s	488.74	Joback Method
dvisc	0.0001965	Pa×s	541.45	Joback Method
dvisc	0.0001347	Pa×s	594.16	Joback Method
dvisc	0.0000982	Pa×s	646.86	Joback Method

dvisc	0.0000751	Pa×s	699.57	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=U292595&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

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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature