o-anisic acid, undec-2-enyl ester

Inchi: InChI=1S/C19H28O3/c1-3-4-5-6-7-8-9-10-13-16-22-19(20)17-14-11-12-15-18(17)21-2/h1
InchiKey: FQNJBJUQBRWUQW-JLHYYAGUSA-N
Formula: C19H28O3
SMILES: CCCCCCCC/C=C/COC(=O)c1ccccc1OC
Mol. weight [g/mol]: 304.43

Physical Properties

Property code	Value	Unit	Source
hf	-528.23	kJ/mol	Cheméo Relay (1.0)
hfus	42.79	kJ/mol	Joback Method
hvap	97.82	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.94		Cheméo Relay (1.0)
logp	5.159		Crippen Method
mcvol	263.820	ml/mol	McGowan Method
pc	1429.38	kPa	Joback Method
rinpol	2310.20		NIST Webbook
tb	619.80	K	Cheméo Relay (1.0)
tc	826.04	K	Cheméo Relay (1.0)
tf	272.52	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.64	J/mol×K	768.65	Joback Method
cpg	861.48	J/mol×K	965.66	Joback Method
cpg	849.17	J/mol×K	932.83	Joback Method
cpg	835.97	J/mol×K	899.99	Joback Method
cpg	821.84	J/mol×K	867.16	Joback Method
cpg	806.77	J/mol×K	834.32	Joback Method
cpg	790.71	J/mol×K	801.49	Joback Method
dvisc	0.0001421	Pa×s	600.39	Joback Method
dvisc	0.0000561	Pa×s	768.65	Joback Method
dvisc	0.0000728	Pa×s	712.57	Joback Method
dvisc	0.0000989	Pa×s	656.48	Joback Method

dvisc	0.0007416	Pa×s	432.14	Joback Method
dvisc	0.0002200	Pa×s	544.31	Joback Method
dvisc	0.0003767	Pa×s	488.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U292578&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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