m-anisic acid, undecyl ester

Other names: m-Anisic acid, undecyl ester
Inchi: InChI=1S/C19H30O3/c1-3-4-5-6-7-8-9-10-11-15-22-19(20)17-13-12-14-18(16-17)21-2/h1
InchiKey: NECXTBYDKQTNTP-UHFFFAOYSA-N
Formula: C19H30O3
SMILES: CCCCCCCCCCCOC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 306.45

Physical Properties

Property code	Value	Unit	Source
af	0.9564		Cheméo Relay (1.0)
hf	-625.42	kJ/mol	Cheméo Relay (1.0)
hfus	42.59	kJ/mol	Joback Method
hvap	99.33	kJ/mol	Cheméo Relay (1.0)
ie	8.60	eV	Cheméo Relay (1.0)
log10ws	-6.29		Cheméo Relay (1.0)
logp	5.383		Crippen Method
mcvol	268.120	ml/mol	McGowan Method
pc	1374.80	kPa	Joback Method
rinpol	2332.80		NIST Webbook
rinpol	2332.80		NIST Webbook
tb	629.20	K	Cheméo Relay (1.0)
tc	822.23	K	Cheméo Relay (1.0)
tf	293.52	K	Cheméo Relay (1.0)
vc	1.017	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.09	J/mol×K	764.49	Joback Method
cpg	815.64	J/mol×K	796.48	Joback Method
cpg	832.16	J/mol×K	828.48	Joback Method
cpg	847.67	J/mol×K	860.47	Joback Method
cpg	862.20	J/mol×K	892.46	Joback Method
cpg	875.75	J/mol×K	924.45	Joback Method

cpg	888.35	J/mol×K	956.45	Joback Method
dvisc	0.0008021	Pa×s	437.22	Joback Method
dvisc	0.0004177	Pa×s	491.76	Joback Method
dvisc	0.0002478	Pa×s	546.31	Joback Method
dvisc	0.0001616	Pa×s	600.86	Joback Method
dvisc	0.0001132	Pa×s	655.40	Joback Method
dvisc	0.0000837	Pa×s	709.94	Joback Method
dvisc	0.0000646	Pa×s	764.49	Joback Method

Sources

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=C69833358&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume