o-Anisic acid, undecyl ester

Inchi: InChI=1S/C19H30O3/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: NDAQNNBMTMMVQB-UHFFFAOYSA-N
Formula: C19H30O3
SMILES: CCCCCCCCCCCOC(=O)c1ccccc1OC
Mol. weight [g/mol]: 306.44

Physical Properties

Property code	Value	Unit	Source
gf	-127.04	kJ/mol	Joback Method
hf	-587.45	kJ/mol	Joback Method
hfus	42.59	kJ/mol	Joback Method
hvap	72.39	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.383		Crippen Method
mcvol	268.120	ml/mol	McGowan Method
pc	1374.80	kPa	Joback Method
rinpol	2279.00		NIST Webbook
rinpol	2279.00		NIST Webbook
tb	764.49	K	Joback Method
tc	956.45	K	Joback Method
tf	437.22	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.09	J/mol×K	764.49	Joback Method
cpg	875.75	J/mol×K	924.45	Joback Method
cpg	862.20	J/mol×K	892.46	Joback Method
cpg	847.67	J/mol×K	860.47	Joback Method
cpg	832.16	J/mol×K	828.48	Joback Method
cpg	815.64	J/mol×K	796.48	Joback Method
cpg	888.35	J/mol×K	956.45	Joback Method
dvisc	0.0000646	Pa×s	764.49	Joback Method

dvisc	0.0000837	Pa×s	709.94	Joback Method
dvisc	0.0001132	Pa×s	655.40	Joback Method
dvisc	0.0001616	Pa×s	600.86	Joback Method
dvisc	0.0002478	Pa×s	546.31	Joback Method
dvisc	0.0004177	Pa×s	491.76	Joback Method
dvisc	0.0008021	Pa×s	437.22	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299951&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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