o-Anisic acid, 2-tridecyl ester

Inchi: InChI=1S/C21H34O3/c1-4-5-6-7-8-9-10-11-12-15-18(2)24-21(22)19-16-13-14-17-20(19)2
InchiKey: ZYWRIFPFSBZDDJ-UHFFFAOYSA-N
Formula: C21H34O3
SMILES: CCCCCCCCCCCC(C)OC(=O)c1ccccc1OC
Mol. weight [g/mol]: 334.49

Physical Properties

Property code	Value	Unit	Source
gf	-112.64	kJ/mol	Joback Method
hf	-634.01	kJ/mol	Joback Method
hfus	44.25	kJ/mol	Joback Method
hvap	76.46	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	6.161		Crippen Method
mcvol	296.300	ml/mol	McGowan Method
pc	1204.80	kPa	Joback Method
rinpol	2362.00		NIST Webbook
rinpol	2362.00		NIST Webbook
tb	809.81	K	Joback Method
tc	1004.18	K	Joback Method
tf	444.76	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.73	J/mol×K	809.81	Joback Method
cpg	996.56	J/mol×K	971.78	Joback Method
cpg	982.77	J/mol×K	939.39	Joback Method
cpg	967.92	J/mol×K	906.99	Joback Method
cpg	951.98	J/mol×K	874.60	Joback Method
cpg	934.92	J/mol×K	842.20	Joback Method
cpg	1009.32	J/mol×K	1004.18	Joback Method
dvisc	0.0000454	Pa×s	809.81	Joback Method

dvisc	0.0000601	Pa×s	748.97	Joback Method
dvisc	0.0000836	Pa×s	688.13	Joback Method
dvisc	0.0001241	Pa×s	627.28	Joback Method
dvisc	0.0002003	Pa×s	566.44	Joback Method
dvisc	0.0003630	Pa×s	505.60	Joback Method
dvisc	0.0007740	Pa×s	444.76	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=U299758&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