o-Anisic acid, 3-tetradecyl ester

Inchi: InChI=1S/C22H36O3/c1-4-6-7-8-9-10-11-12-13-16-19(5-2)25-22(23)20-17-14-15-18-21(2
InchiKey: XENIJNQQROZZDG-UHFFFAOYSA-N
Formula: C22H36O3
SMILES: CCCCCCCCCCCC(CC)OC(=O)c1ccccc1OC
Mol. weight [g/mol]: 348.52

Physical Properties

Property code	Value	Unit	Source
gf	-104.22	kJ/mol	Joback Method
hf	-654.65	kJ/mol	Joback Method
hfus	46.84	kJ/mol	Joback Method
hvap	78.68	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	6.551		Crippen Method
mcvol	310.390	ml/mol	McGowan Method
pc	1128.35	kPa	Joback Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook
tb	832.69	K	Joback Method
tc	1028.10	K	Joback Method
tf	456.03	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.05	J/mol×K	832.69	Joback Method
cpg	1057.51	J/mol×K	995.53	Joback Method
cpg	1043.67	J/mol×K	962.96	Joback Method
cpg	1028.73	J/mol×K	930.39	Joback Method
cpg	1012.66	J/mol×K	897.83	Joback Method
cpg	995.45	J/mol×K	865.26	Joback Method
cpg	1070.27	J/mol×K	1028.10	Joback Method
dvisc	0.0000395	Pa×s	832.69	Joback Method

dvisc	0.0000524	Pa×s	769.91	Joback Method
dvisc	0.0000731	Pa×s	707.14	Joback Method
dvisc	0.0001089	Pa×s	644.36	Joback Method
dvisc	0.0001769	Pa×s	581.58	Joback Method
dvisc	0.0003228	Pa×s	518.81	Joback Method
dvisc	0.0006955	Pa×s	456.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299762&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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