p-Methoxybenzoic acid, tetradecyl ester

Inchi: InChI=1S/C22H36O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-19-25-22(23)20-15-17-21(24-2)18
InchiKey: WFEHAGGZQNLTCA-UHFFFAOYSA-N
Formula: C22H36O3
SMILES: CCCCCCCCCCCCCCOC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 348.52
CAS: 111722-07-7

Physical Properties

Property code	Value	Unit	Source
gf	-101.78	kJ/mol	Joback Method
hf	-649.37	kJ/mol	Joback Method
hfus	50.36	kJ/mol	Joback Method
hvap	79.07	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	6.553		Crippen Method
mcvol	310.390	ml/mol	McGowan Method
pc	1122.31	kPa	Joback Method
rinpol	2694.10		NIST Webbook
rinpol	2694.10		NIST Webbook
tb	833.13	K	Joback Method
tc	1027.17	K	Joback Method
tf	471.03	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.56	J/mol×K	833.13	Joback Method
cpg	1056.67	J/mol×K	994.83	Joback Method
cpg	1042.85	J/mol×K	962.49	Joback Method
cpg	1027.96	J/mol×K	930.15	Joback Method
cpg	1011.96	J/mol×K	897.81	Joback Method
cpg	994.84	J/mol×K	865.47	Joback Method
cpg	1069.44	J/mol×K	1027.17	Joback Method

dvisc	0.0000431	Pa×s	833.13	Joback Method
dvisc	0.0000563	Pa×s	772.78	Joback Method
dvisc	0.0000769	Pa×s	712.43	Joback Method
dvisc	0.0001115	Pa×s	652.08	Joback Method
dvisc	0.0001742	Pa×s	591.73	Joback Method
dvisc	0.0003013	Pa×s	531.38	Joback Method
dvisc	0.0005996	Pa×s	471.03	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111722077&Units=SI

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