p-Anisic acid, 4-hexadecyl ester

Inchi: InChI=1S/C24H40O3/c1-4-6-7-8-9-10-11-12-13-14-16-23(15-5-2)27-24(25)21-17-19-22(2
InchiKey: ZSQPHXQMQBANPM-UHFFFAOYSA-N
Formula: C24H40O3
SMILES: CCCCCCCCCCCCCC(CCC)OC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 376.57

Physical Properties

Property code	Value	Unit	Source
gf	-87.38	kJ/mol	Joback Method
hf	-695.93	kJ/mol	Joback Method
hfus	52.02	kJ/mol	Joback Method
hvap	83.13	kJ/mol	Joback Method
log10ws	-8.22		Crippen Method
logp	7.332		Crippen Method
mcvol	338.570	ml/mol	McGowan Method
pc	995.76	kPa	Joback Method
rinpol	2546.20		NIST Webbook
rinpol	2546.20		NIST Webbook
tb	878.45	K	Joback Method
tc	1078.15	K	Joback Method
tf	478.57	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1099.82	J/mol×K	878.45	Joback Method
cpg	1181.51	J/mol×K	1044.87	Joback Method
cpg	1167.62	J/mol×K	1011.59	Joback Method
cpg	1152.53	J/mol×K	978.30	Joback Method
cpg	1136.23	J/mol×K	945.02	Joback Method
cpg	1118.67	J/mol×K	911.73	Joback Method
cpg	1194.26	J/mol×K	1078.15	Joback Method
dvisc	0.0000296	Pa×s	878.45	Joback Method

dvisc	0.0000395	Pa×s	811.80	Joback Method
dvisc	0.0000555	Pa×s	745.16	Joback Method
dvisc	0.0000833	Pa×s	678.51	Joback Method
dvisc	0.0001365	Pa×s	611.86	Joback Method
dvisc	0.0002526	Pa×s	545.22	Joback Method
dvisc	0.0005549	Pa×s	478.57	Joback Method

Sources

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=U292462&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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