p-Methoxybenzoic acid, hexadecyl ester

Inchi: InChI=1S/C24H40O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-27-24(25)22-17-19-23(2
InchiKey: BGDWOWNIOQVMOB-UHFFFAOYSA-N
Formula: C24H40O3
SMILES: CCCCCCCCCCCCCCCCOC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 376.57
CAS: 111722-13-5

Physical Properties

Property code	Value	Unit	Source
gf	-84.94	kJ/mol	Joback Method
hf	-690.65	kJ/mol	Joback Method
hfus	55.54	kJ/mol	Joback Method
hvap	83.52	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.333		Crippen Method
mcvol	338.570	ml/mol	McGowan Method
pc	990.75	kPa	Joback Method
rinpol	2885.00		NIST Webbook
rinpol	2885.00		NIST Webbook
tb	878.89	K	Joback Method
tc	1077.89	K	Joback Method
tf	493.57	K	Joback Method
vc	1.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1099.37	J/mol×K	878.89	Joback Method
cpg	1181.02	J/mol×K	1044.73	Joback Method
cpg	1167.09	J/mol×K	1011.56	Joback Method
cpg	1152.00	J/mol×K	978.39	Joback Method
cpg	1135.70	J/mol×K	945.22	Joback Method
cpg	1118.17	J/mol×K	912.06	Joback Method
cpg	1193.81	J/mol×K	1077.89	Joback Method

dvisc	0.0000324	Pa×s	878.89	Joback Method
dvisc	0.0000425	Pa×s	814.67	Joback Method
dvisc	0.0000586	Pa×s	750.45	Joback Method
dvisc	0.0000856	Pa×s	686.23	Joback Method
dvisc	0.0001353	Pa×s	622.01	Joback Method
dvisc	0.0002376	Pa×s	557.79	Joback Method
dvisc	0.0004833	Pa×s	493.57	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=C111722135&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