o-Toluic acid, hexadecyl ester

Other names: o-Toluylic acid, hexadecyl ester
Inchi: InChI=1S/C24H40O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-26-24(25)23-20-17-16-1
InchiKey: QUDQJCHCKASANX-UHFFFAOYSA-N
Formula: C24H40O2
SMILES: CCCCCCCCCCCCCCCCOC(=O)c1ccccc1C
Mol. weight [g/mol]: 360.57

Physical Properties

Property code	Value	Unit	Source
gf	20.06	kJ/mol	Joback Method
hf	-558.43	kJ/mol	Joback Method
hfus	54.35	kJ/mol	Joback Method
hvap	81.11	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	7.633		Crippen Method
mcvol	332.700	ml/mol	McGowan Method
pc	1001.44	kPa	Joback Method
rinpol	2644.90		NIST Webbook
rinpol	2644.90		NIST Webbook
tb	856.47	K	Joback Method
tc	1052.40	K	Joback Method
tf	471.34	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.56	J/mol×K	856.47	Joback Method
cpg	1086.77	J/mol×K	889.13	Joback Method
cpg	1104.80	J/mol×K	921.78	Joback Method
cpg	1121.70	J/mol×K	954.44	Joback Method
cpg	1137.51	J/mol×K	987.09	Joback Method
cpg	1152.27	J/mol×K	1019.75	Joback Method
cpg	1166.02	J/mol×K	1052.40	Joback Method

dvisc	0.0007027	Pa×s	471.34	Joback Method
dvisc	0.0003343	Pa×s	535.53	Joback Method
dvisc	0.0001865	Pa×s	599.72	Joback Method
dvisc	0.0001165	Pa×s	663.90	Joback Method
dvisc	0.0000790	Pa×s	728.09	Joback Method
dvisc	0.0000571	Pa×s	792.28	Joback Method
dvisc	0.0000433	Pa×s	856.47	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=U292385&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