Hexadecyl p-toluate

Other names: Benzoic Acid, 4-methyl, hexadecyl ester
p-Toluylic acid, hexadecyl ester
Inchi: InChI=1S/C24H40O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-26-24(25)23-19-17-22(2
InchiKey: HOZUXBBJIHXFNR-UHFFFAOYSA-N
Formula: C24H40O2
SMILES: CCCCCCCCCCCCCCCCOC(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 360.57
CAS: 959083-37-5

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	2730.20		NIST Webbook
rinpol	2730.20		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: 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=C959083375&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