Benzoic acid, 4-tert-butyl-, tetradecyl ester

Inchi: InChI=1S/C25H42O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-21-27-24(26)22-17-19-23(20-1
InchiKey: CGLITVALXPCPLD-UHFFFAOYSA-N
Formula: C25H42O2
SMILES: CCCCCCCCCCCCCCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 374.60

Physical Properties

Property code	Value	Unit	Source
gf	31.32	kJ/mol	Joback Method
hf	-587.82	kJ/mol	Joback Method
hfus	49.53	kJ/mol	Joback Method
hvap	82.04	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	7.842		Crippen Method
mcvol	346.790	ml/mol	McGowan Method
pc	954.37	kPa	Joback Method
rinpol	2786.00		NIST Webbook
tb	876.12	K	Joback Method
tc	1076.98	K	Joback Method
tf	485.03	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1130.09	J/mol×K	876.12	Joback Method
cpg	1216.35	J/mol×K	1043.50	Joback Method
cpg	1201.24	J/mol×K	1010.02	Joback Method
cpg	1185.13	J/mol×K	976.55	Joback Method
cpg	1167.94	J/mol×K	943.07	Joback Method
cpg	1149.62	J/mol×K	909.60	Joback Method
cpg	1230.51	J/mol×K	1076.98	Joback Method
dvisc	0.0000293	Pa×s	876.12	Joback Method
dvisc	0.0000396	Pa×s	810.94	Joback Method

dvisc	0.0000562	Pa×s	745.76	Joback Method
dvisc	0.0000853	Pa×s	680.58	Joback Method
dvisc	0.0001417	Pa×s	615.39	Joback Method
dvisc	0.0002651	Pa×s	550.21	Joback Method
dvisc	0.0005871	Pa×s	485.03	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=U406150&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