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

Inchi: InChI=1S/C24H40O2/c1-5-6-7-8-9-10-11-12-13-14-15-20-26-23(25)21-16-18-22(19-17-2
InchiKey: MCMOTKKJQLDYFX-UHFFFAOYSA-N
Formula: C24H40O2
SMILES: CCCCCCCCCCCCCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 360.57

Physical Properties

Property code	Value	Unit	Source
gf	22.90	kJ/mol	Joback Method
hf	-567.18	kJ/mol	Joback Method
hfus	46.94	kJ/mol	Joback Method
hvap	79.82	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	7.452		Crippen Method
mcvol	332.700	ml/mol	McGowan Method
pc	1013.59	kPa	Joback Method
rinpol	2684.00		NIST Webbook
rinpol	2684.00		NIST Webbook
tb	853.24	K	Joback Method
tc	1052.12	K	Joback Method
tf	473.76	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1068.08	J/mol×K	853.24	Joback Method
cpg	1087.37	J/mol×K	886.39	Joback Method
cpg	1105.48	J/mol×K	919.53	Joback Method
cpg	1122.48	J/mol×K	952.68	Joback Method
cpg	1138.42	J/mol×K	985.83	Joback Method
cpg	1153.37	J/mol×K	1018.98	Joback Method
cpg	1167.40	J/mol×K	1052.12	Joback Method
dvisc	0.0006631	Pa×s	473.76	Joback Method

dvisc	0.0003022	Pa×s	537.01	Joback Method
dvisc	0.0001625	Pa×s	600.25	Joback Method
dvisc	0.0000984	Pa×s	663.50	Joback Method
dvisc	0.0000650	Pa×s	726.75	Joback Method
dvisc	0.0000459	Pa×s	789.99	Joback Method
dvisc	0.0000341	Pa×s	853.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406149&Units=SI
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

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