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

Inchi: InChI=1S/C22H36O2/c1-5-6-7-8-9-10-11-12-13-18-24-21(23)19-14-16-20(17-15-19)22(2
InchiKey: XNTOKZLDGKOLNM-UHFFFAOYSA-N
Formula: C22H36O2
SMILES: CCCCCCCCCCCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 332.52

Physical Properties

Property code	Value	Unit	Source
gf	6.06	kJ/mol	Joback Method
hf	-525.90	kJ/mol	Joback Method
hfus	41.76	kJ/mol	Joback Method
hvap	75.36	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	6.672		Crippen Method
mcvol	304.520	ml/mol	McGowan Method
pc	1149.87	kPa	Joback Method
rinpol	2476.00		NIST Webbook
rinpol	2476.00		NIST Webbook
tb	807.48	K	Joback Method
tc	1004.62	K	Joback Method
tf	451.22	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	946.21	J/mol×K	807.48	Joback Method
cpg	1029.87	J/mol×K	971.77	Joback Method
cpg	1015.19	J/mol×K	938.91	Joback Method
cpg	999.53	J/mol×K	906.05	Joback Method
cpg	982.86	J/mol×K	873.19	Joback Method
cpg	965.10	J/mol×K	840.34	Joback Method
cpg	1043.63	J/mol×K	1004.62	Joback Method
dvisc	0.0000457	Pa×s	807.48	Joback Method

dvisc	0.0000613	Pa×s	748.10	Joback Method
dvisc	0.0000863	Pa×s	688.73	Joback Method
dvisc	0.0001297	Pa×s	629.35	Joback Method
dvisc	0.0002121	Pa×s	569.97	Joback Method
dvisc	0.0003891	Pa×s	510.60	Joback Method
dvisc	0.0008371	Pa×s	451.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406147&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