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

Inchi: InChI=1S/C21H34O2/c1-5-6-7-8-9-10-11-12-17-23-20(22)18-13-15-19(16-14-18)21(2,3)4
InchiKey: KDPKSPVSWJHSDT-UHFFFAOYSA-N
Formula: C21H34O2
SMILES: CCCCCCCCCCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 318.49

Physical Properties

Property code	Value	Unit	Source
gf	-2.36	kJ/mol	Joback Method
hf	-505.26	kJ/mol	Joback Method
hfus	39.17	kJ/mol	Joback Method
hvap	73.14	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	6.282		Crippen Method
mcvol	290.430	ml/mol	McGowan Method
pc	1228.56	kPa	Joback Method
rinpol	2368.00		NIST Webbook
rinpol	2368.00		NIST Webbook
tb	784.60	K	Joback Method
tc	981.87	K	Joback Method
tf	439.95	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.47	J/mol×K	784.60	Joback Method
cpg	905.19	J/mol×K	817.48	Joback Method
cpg	922.78	J/mol×K	850.36	Joback Method
cpg	939.31	J/mol×K	883.23	Joback Method
cpg	954.82	J/mol×K	916.11	Joback Method
cpg	969.37	J/mol×K	948.99	Joback Method
cpg	983.01	J/mol×K	981.87	Joback Method
dvisc	0.0009350	Pa×s	439.95	Joback Method

dvisc	0.0004392	Pa×s	497.39	Joback Method
dvisc	0.0002412	Pa×s	554.83	Joback Method
dvisc	0.0001483	Pa×s	612.27	Joback Method
dvisc	0.0000991	Pa×s	669.72	Joback Method
dvisc	0.0000705	Pa×s	727.16	Joback Method
dvisc	0.0000528	Pa×s	784.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406146&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