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

Inchi: InChI=1S/C28H48O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-24-30-27(29)25-20-2
InchiKey: OKNBIEFPBAWQLK-UHFFFAOYSA-N
Formula: C28H48O2
SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 416.68

Physical Properties

Property code	Value	Unit	Source
gf	56.58	kJ/mol	Joback Method
hf	-649.74	kJ/mol	Joback Method
hfus	57.30	kJ/mol	Joback Method
hvap	88.72	kJ/mol	Joback Method
log10ws	-9.73		Crippen Method
logp	9.012		Crippen Method
mcvol	389.060	ml/mol	McGowan Method
pc	804.79	kPa	Joback Method
rinpol	3093.00		NIST Webbook
rinpol	3093.00		NIST Webbook
tb	944.76	K	Joback Method
tc	1156.65	K	Joback Method
tf	518.84	K	Joback Method
vc	1.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1319.80	J/mol×K	944.76	Joback Method
cpg	1340.32	J/mol×K	980.08	Joback Method
cpg	1359.50	J/mol×K	1015.39	Joback Method
cpg	1377.44	J/mol×K	1050.71	Joback Method
cpg	1394.22	J/mol×K	1086.02	Joback Method
cpg	1409.94	J/mol×K	1121.34	Joback Method
cpg	1424.67	J/mol×K	1156.65	Joback Method
dvisc	0.0004001	Pa×s	518.84	Joback Method

dvisc	0.0001761	Pa×s	589.83	Joback Method
dvisc	0.0000925	Pa×s	660.81	Joback Method
dvisc	0.0000550	Pa×s	731.80	Joback Method
dvisc	0.0000359	Pa×s	802.79	Joback Method
dvisc	0.0000251	Pa×s	873.77	Joback Method
dvisc	0.0000185	Pa×s	944.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406153&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

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