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

Inchi: InChI=1S/C18H28O2/c1-5-6-7-8-9-14-20-17(19)15-10-12-16(13-11-15)18(2,3)4/h10-13H
InchiKey: FHHQGIUYESVIDK-UHFFFAOYSA-N
Formula: C18H28O2
SMILES: CCCCCCCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 276.41

Physical Properties

Property code	Value	Unit	Source
gf	-27.62	kJ/mol	Joback Method
hf	-443.34	kJ/mol	Joback Method
hfus	31.40	kJ/mol	Joback Method
hvap	66.46	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.111		Crippen Method
mcvol	248.160	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
rinpol	2058.00		NIST Webbook
rinpol	2058.00		NIST Webbook
tb	715.96	K	Joback Method
tc	916.98	K	Joback Method
tf	406.14	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.79	J/mol×K	715.96	Joback Method
cpg	730.94	J/mol×K	749.46	Joback Method
cpg	748.01	J/mol×K	782.97	Joback Method
cpg	764.02	J/mol×K	816.47	Joback Method
cpg	779.05	J/mol×K	849.97	Joback Method
cpg	793.12	J/mol×K	883.47	Joback Method
cpg	806.30	J/mol×K	916.98	Joback Method
dvisc	0.0012678	Pa×s	406.14	Joback Method

dvisc	0.0006164	Pa×s	457.78	Joback Method
dvisc	0.0003469	Pa×s	509.41	Joback Method
dvisc	0.0002170	Pa×s	561.05	Joback Method
dvisc	0.0001469	Pa×s	612.69	Joback Method
dvisc	0.0001057	Pa×s	664.32	Joback Method
dvisc	0.0000797	Pa×s	715.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406143&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

Latest version available from:
https://www.chemeo.com/cid/89-284-9/Benzoic-acid-4-tert-butyl-heptyl-ester.pdf
Generated by Cheméo on 2025-12-25 00:41:30.036944077 +0000 UTC m=+6371487.566984732.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.