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

Other names: Hexyl 4-tert-butyl benzoate
Inchi: InChI=1S/C17H26O2/c1-5-6-7-8-13-19-16(18)14-9-11-15(12-10-14)17(2,3)4/h9-12H,5-8,
InchiKey: UDLBJVKJBFYKBU-UHFFFAOYSA-N
Formula: C17H26O2
SMILES: CCCCCCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	-36.04	kJ/mol	Joback Method
hf	-422.70	kJ/mol	Joback Method
hfus	28.81	kJ/mol	Joback Method
hvap	64.23	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.721		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	1892.00		NIST Webbook
rinpol	1892.00		NIST Webbook
rinpol	1952.00		NIST Webbook
rinpol	1952.00		NIST Webbook
tb	693.08	K	Joback Method
tc	896.32	K	Joback Method
tf	394.87	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.98	J/mol×K	693.08	Joback Method
cpg	736.20	J/mol×K	862.45	Joback Method
cpg	722.34	J/mol×K	828.57	Joback Method
cpg	707.53	J/mol×K	794.70	Joback Method
cpg	691.73	J/mol×K	760.83	Joback Method

cpg	674.90	J/mol×K	726.95	Joback Method
cpg	749.17	J/mol×K	896.32	Joback Method
dvisc	0.0000909	Pa×s	693.08	Joback Method
dvisc	0.0001201	Pa×s	643.38	Joback Method
dvisc	0.0001663	Pa×s	593.68	Joback Method
dvisc	0.0002445	Pa×s	543.97	Joback Method
dvisc	0.0003882	Pa×s	494.27	Joback Method
dvisc	0.0006837	Pa×s	444.57	Joback Method
dvisc	0.0013885	Pa×s	394.87	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406142&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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