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

Inchi: InChI=1S/C16H24O2/c1-5-6-7-12-18-15(17)13-8-10-14(11-9-13)16(2,3)4/h8-11H,5-7,12H
InchiKey: NMZMYUFNTICNPP-UHFFFAOYSA-N
Formula: C16H24O2
SMILES: CCCCCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	-44.46	kJ/mol	Joback Method
hf	-402.06	kJ/mol	Joback Method
hfus	26.22	kJ/mol	Joback Method
hvap	62.01	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.331		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	1848.00		NIST Webbook
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tb	670.20	K	Joback Method
tc	876.07	K	Joback Method
tf	383.60	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.34	J/mol×K	670.20	Joback Method
cpg	680.24	J/mol×K	841.76	Joback Method
cpg	666.62	J/mol×K	807.45	Joback Method
cpg	652.07	J/mol×K	773.14	Joback Method
cpg	636.53	J/mol×K	738.82	Joback Method
cpg	619.97	J/mol×K	704.51	Joback Method
cpg	692.96	J/mol×K	876.07	Joback Method
dvisc	0.0001032	Pa×s	670.20	Joback Method

dvisc	0.0001359	Pa×s	622.43	Joback Method
dvisc	0.0001875	Pa×s	574.67	Joback Method
dvisc	0.0002741	Pa×s	526.90	Joback Method
dvisc	0.0004323	Pa×s	479.13	Joback Method
dvisc	0.0007542	Pa×s	431.37	Joback Method
dvisc	0.0015113	Pa×s	383.60	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406141&Units=SI

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