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

Inchi: InChI=1S/C27H46O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23-29-26(28)24-19-21-2
InchiKey: WORLJKXGDQDFSS-UHFFFAOYSA-N
Formula: C27H46O2
SMILES: CCCCCCCCCCCCCCCCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 402.65

Physical Properties

Property code	Value	Unit	Source
gf	48.16	kJ/mol	Joback Method
hf	-629.10	kJ/mol	Joback Method
hfus	54.71	kJ/mol	Joback Method
hvap	86.49	kJ/mol	Joback Method
log10ws	-9.31		Crippen Method
logp	8.622		Crippen Method
mcvol	374.970	ml/mol	McGowan Method
pc	850.48	kPa	Joback Method
rinpol	2988.00		NIST Webbook
rinpol	2988.00		NIST Webbook
tb	921.88	K	Joback Method
tc	1129.18	K	Joback Method
tf	507.57	K	Joback Method
vc	1.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.00	J/mol×K	921.88	Joback Method
cpg	1276.13	J/mol×K	956.43	Joback Method
cpg	1294.98	J/mol×K	990.98	Joback Method
cpg	1312.63	J/mol×K	1025.53	Joback Method
cpg	1329.16	J/mol×K	1060.08	Joback Method
cpg	1344.64	J/mol×K	1094.63	Joback Method
cpg	1359.15	J/mol×K	1129.18	Joback Method
dvisc	0.0004559	Pa×s	507.57	Joback Method

dvisc	0.0002023	Pa×s	576.62	Joback Method
dvisc	0.0001068	Pa×s	645.67	Joback Method
dvisc	0.0000638	Pa×s	714.72	Joback Method
dvisc	0.0000417	Pa×s	783.78	Joback Method
dvisc	0.0000292	Pa×s	852.83	Joback Method
dvisc	0.0000216	Pa×s	921.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406152&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