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

Inchi: InChI=1S/C19H30O2/c1-5-6-7-8-9-10-15-21-18(20)16-11-13-17(14-12-16)19(2,3)4/h11-1
InchiKey: LYHCEGUOXQINQJ-UHFFFAOYSA-N
Formula: C19H30O2
SMILES: CCCCCCCCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 290.44

Physical Properties

Property code	Value	Unit	Source
gf	-19.20	kJ/mol	Joback Method
hf	-463.98	kJ/mol	Joback Method
hfus	33.99	kJ/mol	Joback Method
hvap	68.69	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.501		Crippen Method
mcvol	262.250	ml/mol	McGowan Method
pc	1412.25	kPa	Joback Method
rinpol	2162.00		NIST Webbook
rinpol	2162.00		NIST Webbook
tb	738.84	K	Joback Method
tc	938.09	K	Joback Method
tf	417.41	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.69	J/mol×K	738.84	Joback Method
cpg	850.97	J/mol×K	904.88	Joback Method
cpg	836.72	J/mol×K	871.67	Joback Method
cpg	821.51	J/mol×K	838.47	Joback Method
cpg	805.31	J/mol×K	805.26	Joback Method
cpg	788.05	J/mol×K	772.05	Joback Method
cpg	864.33	J/mol×K	938.09	Joback Method
dvisc	0.0000697	Pa×s	738.84	Joback Method

dvisc	0.0000927	Pa×s	685.27	Joback Method
dvisc	0.0001293	Pa×s	631.70	Joback Method
dvisc	0.0001918	Pa×s	578.12	Joback Method
dvisc	0.0003086	Pa×s	524.55	Joback Method
dvisc	0.0005530	Pa×s	470.98	Joback Method
dvisc	0.0011512	Pa×s	417.41	Joback Method

Sources

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=U406144&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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