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

Inchi: InChI=1S/C29H50O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-25-31-28(30)26-2
InchiKey: LOEGNUHLVGAMMW-UHFFFAOYSA-N
Formula: C29H50O2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 430.71

Physical Properties

Property code	Value	Unit	Source
gf	65.00	kJ/mol	Joback Method
hf	-670.38	kJ/mol	Joback Method
hfus	59.89	kJ/mol	Joback Method
hvap	90.95	kJ/mol	Joback Method
log10ws	-10.14		Crippen Method
logp	9.402		Crippen Method
mcvol	403.150	ml/mol	McGowan Method
pc	762.68	kPa	Joback Method
rinpol	3203.00		NIST Webbook
rinpol	3203.00		NIST Webbook
tb	967.64	K	Joback Method
tc	1185.14	K	Joback Method
tf	530.11	K	Joback Method
vc	1.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.11	J/mol×K	967.64	Joback Method
cpg	1405.07	J/mol×K	1003.89	Joback Method
cpg	1424.64	J/mol×K	1040.14	Joback Method
cpg	1442.91	J/mol×K	1076.39	Joback Method
cpg	1460.00	J/mol×K	1112.64	Joback Method
cpg	1475.99	J/mol×K	1148.89	Joback Method
cpg	1490.98	J/mol×K	1185.14	Joback Method
dvisc	0.0003502	Pa×s	530.11	Joback Method

dvisc	0.0001529	Pa×s	603.03	Joback Method
dvisc	0.0000799	Pa×s	675.95	Joback Method
dvisc	0.0000473	Pa×s	748.88	Joback Method
dvisc	0.0000308	Pa×s	821.80	Joback Method
dvisc	0.0000215	Pa×s	894.72	Joback Method
dvisc	0.0000158	Pa×s	967.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406154&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