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

Inchi: InChI=1S/C26H44O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-22-28-25(27)23-18-20-24(2
InchiKey: VWYKFDOLYZLSLQ-UHFFFAOYSA-N
Formula: C26H44O2
SMILES: CCCCCCCCCCCCCCCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 388.63

Physical Properties

Property code	Value	Unit	Source
gf	39.74	kJ/mol	Joback Method
hf	-608.46	kJ/mol	Joback Method
hfus	52.12	kJ/mol	Joback Method
hvap	84.27	kJ/mol	Joback Method
log10ws	-8.89		Crippen Method
logp	8.232		Crippen Method
mcvol	360.880	ml/mol	McGowan Method
pc	900.18	kPa	Joback Method
rinpol	2883.00		NIST Webbook
rinpol	2883.00		NIST Webbook
tb	899.00	K	Joback Method
tc	1102.64	K	Joback Method
tf	496.30	K	Joback Method
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1192.75	J/mol×K	899.00	Joback Method
cpg	1212.55	J/mol×K	932.94	Joback Method
cpg	1231.12	J/mol×K	966.88	Joback Method
cpg	1248.52	J/mol×K	1000.82	Joback Method
cpg	1264.82	J/mol×K	1034.76	Joback Method
cpg	1280.11	J/mol×K	1068.70	Joback Method
cpg	1294.43	J/mol×K	1102.64	Joback Method
dvisc	0.0005181	Pa×s	496.30	Joback Method

dvisc	0.0002319	Pa×s	563.42	Joback Method
dvisc	0.0001232	Pa×s	630.53	Joback Method
dvisc	0.0000739	Pa×s	697.65	Joback Method
dvisc	0.0000485	Pa×s	764.77	Joback Method
dvisc	0.0000340	Pa×s	831.88	Joback Method
dvisc	0.0000252	Pa×s	899.00	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=U406151&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