2-Ethylhexyl 4-tert-butylbenzoate

Inchi: InChI=1S/C19H30O2/c1-6-8-9-15(7-2)14-21-18(20)16-10-12-17(13-11-16)19(3,4)5/h10-1
InchiKey: SBTSOUSSYNGQHT-UHFFFAOYSA-N
Formula: C19H30O2
SMILES: CCCCC(CC)COC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 290.44

Physical Properties

Property code	Value	Unit	Source
gf	-21.64	kJ/mol	Joback Method
hf	-469.26	kJ/mol	Joback Method
hfus	30.47	kJ/mol	Joback Method
hvap	68.30	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	5.357		Crippen Method
mcvol	262.250	ml/mol	McGowan Method
pc	1420.78	kPa	Joback Method
rinpol	2019.00		NIST Webbook
tb	738.40	K	Joback Method
tc	940.58	K	Joback Method
tf	402.41	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.19	J/mol×K	738.40	Joback Method
cpg	788.83	J/mol×K	772.10	Joback Method
cpg	806.32	J/mol×K	805.79	Joback Method
cpg	822.73	J/mol×K	839.49	Joback Method
cpg	838.10	J/mol×K	873.18	Joback Method
cpg	852.48	J/mol×K	906.88	Joback Method
cpg	865.93	J/mol×K	940.58	Joback Method
dvisc	0.0014064	Pa×s	402.41	Joback Method
dvisc	0.0006144	Pa×s	458.41	Joback Method

dvisc	0.0003214	Pa×s	514.41	Joback Method
dvisc	0.0001909	Pa×s	570.40	Joback Method
dvisc	0.0001245	Pa×s	626.40	Joback Method
dvisc	0.0000871	Pa×s	682.40	Joback Method
dvisc	0.0000643	Pa×s	738.40	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=R540331&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