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

Inchi: InChI=1S/C20H32O2/c1-5-6-7-8-9-10-11-16-22-19(21)17-12-14-18(15-13-17)20(2,3)4/h1
InchiKey: MUZHGYBPDHHONZ-UHFFFAOYSA-N
Formula: C20H32O2
SMILES: CCCCCCCCCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 304.47

Physical Properties

Property code	Value	Unit	Source
gf	-10.78	kJ/mol	Joback Method
hf	-484.62	kJ/mol	Joback Method
hfus	36.58	kJ/mol	Joback Method
hvap	70.91	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.891		Crippen Method
mcvol	276.340	ml/mol	McGowan Method
pc	1315.61	kPa	Joback Method
rinpol	2267.00		NIST Webbook
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tb	761.72	K	Joback Method
tc	959.70	K	Joback Method
tf	428.68	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.61	J/mol×K	761.72	Joback Method
cpg	909.73	J/mol×K	926.71	Joback Method
cpg	895.32	J/mol×K	893.71	Joback Method
cpg	879.95	J/mol×K	860.71	Joback Method
cpg	863.58	J/mol×K	827.71	Joback Method
cpg	846.15	J/mol×K	794.72	Joback Method
cpg	923.23	J/mol×K	959.70	Joback Method
dvisc	0.0000608	Pa×s	761.72	Joback Method

dvisc	0.0000810	Pa×s	706.21	Joback Method
dvisc	0.0001133	Pa×s	650.71	Joback Method
dvisc	0.0001689	Pa×s	595.20	Joback Method
dvisc	0.0002733	Pa×s	539.69	Joback Method
dvisc	0.0004938	Pa×s	484.19	Joback Method
dvisc	0.0010399	Pa×s	428.68	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=U406145&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