Benzoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester

Othernames:	Benzoic acid, 3,5-di-tert-butyl-4-hydroxy-, methyl ester
	Methyl 3,5-di-tert-butyl-4-hydroxybenzoate
	3,5-Di-tert-butyl-4-hydroxybenzoic acid, methyl ester
	Benzoic acid, 4-hydroxy-3,5-di-tert-butyl, methyl ester
	Benzoic acid, 4-hydroxy-3,5-di-tert.-butyl, methyl ester
	methyl 3,5-bis-tert-butyl-4-hydroxybenzoate
Inchi:	InChI=1S/C16H24O3/c1-15(2,3)11-8-10(14(18)19-7)9-12(13(11)17)16(4,5)6/h8-9,17H,1-
InchiKey:	UPVYFJALDJUSOV-UHFFFAOYSA-N
Formula:	C16H24O3
SMILES:	COC(=O)c1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]:	264.36
CAS:	2511-22-0

Physical Properties

Property code	Value	Unit	Source
gf	-205.87	kJ/mol	Joback Method
hf	-599.59	kJ/mol	Joback Method
hfus	24.20	kJ/mol	Joback Method
hvap	74.39	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.774		Crippen Method
mcvol	225.850	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	1859.30		NIST Webbook
rinpol	1859.30		NIST Webbook
rinpol	1872.00		NIST Webbook
rinpol	1872.00		NIST Webbook
tb	752.57	K	Joback Method
tc	978.28	K	Joback Method
tf	510.26	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.31	J/mol×K	752.57	Joback Method
cpg	678.30	J/mol×K	790.19	Joback Method
cpg	693.33	J/mol×K	827.81	Joback Method
cpg	707.50	J/mol×K	865.42	Joback Method
cpg	720.95	J/mol×K	903.04	Joback Method
cpg	733.78	J/mol×K	940.66	Joback Method
cpg	746.11	J/mol×K	978.28	Joback Method
dvisc	0.0001455	Pa×s	510.26	Joback Method
dvisc	0.0000698	Pa×s	550.64	Joback Method
dvisc	0.0000370	Pa×s	591.03	Joback Method
dvisc	0.0000213	Pa×s	631.41	Joback Method
dvisc	0.0000131	Pa×s	671.80	Joback Method
dvisc	0.0000085	Pa×s	712.19	Joback Method
dvisc	0.0000058	Pa×s	752.57	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2511220&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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