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

Other names: Benzoic acid, 3,5-di-tert-butyl-4-hydroxy-
3,5-Di-tert-butyl-4-hydroxybenzoic acid
3,5-di-t-Butyl-4-hydroxy benzoic acid
3,5-bis-tert-butyl-4-hydroxybenzoic acid

Inchi: InChI=1S/C15H22O3/c1-14(2,3)10-7-9(13(17)18)8-11(12(10)16)15(4,5)6/h7-8,16H,1-6H3

InchiKey: YEXOWHQZWLCHHD-UHFFFAOYSA-N

Formula: C15H22O3

SMILES: CC(C)(C)c1cc(C(=O)O)cc(C(C)(C)C)c1O

Mol. weight [g/mol]: 250.33

CAS: 1421-49-4

Physical Properties

Property code	Value	Unit	Source
gf	-246.11	kJ/mol	Joback Method
hf	-598.96	kJ/mol	Joback Method
hfus	24.51	kJ/mol	Joback Method
hvap	86.43	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.685		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1924.70		NIST Webbook
rinpol	1924.70		NIST Webbook
tb	799.45	K	Joback Method
tc	1016.79	K	Joback Method
tf	537.58	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.85	J/mol×K	799.45	Joback Method
cpg	648.88	J/mol×K	835.67	Joback Method
cpg	661.26	J/mol×K	871.90	Joback Method

cpg	673.11	J/mol×K	908.12	Joback Method
cpg	684.56	J/mol×K	944.34	Joback Method
cpg	695.72	J/mol×K	980.56	Joback Method
cpg	706.71	J/mol×K	1016.79	Joback Method
dvisc	0.0000709	Pa×s	537.58	Joback Method
dvisc	0.0000282	Pa×s	581.23	Joback Method
dvisc	0.0000127	Pa×s	624.87	Joback Method
dvisc	0.0000064	Pa×s	668.51	Joback Method
dvisc	0.0000035	Pa×s	712.16	Joback Method
dvisc	0.0000020	Pa×s	755.80	Joback Method
dvisc	0.0000013	Pa×s	799.45	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=C1421494&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