3,5-DI-t-BUTYL-4-HYDROXYBENZOIC ACID

Other names:	3,5-Di-tert-butyl-4-hydroxybenzoic acid
	3,5-bis-tert-butyl-4-hydroxybenzoic acid
	3,5-di-t-Butyl-4-hydroxy benzoic acid
	Benzoic acid, 3,5-di-tert-butyl-4-hydroxy-
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]:	250.34

Physical Properties

Property code	Value	Unit	Source
hf	-651.00	kJ/mol	Cheméo Relay (1.0)
hfus	24.51	kJ/mol	Joback Method
hvap	112.69	kJ/mol	Cheméo Relay (1.0)
ie	8.30	eV	Cheméo Relay (1.0)
log10ws	-4.25		Cheméo Relay (1.0)
logp	3.685		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
rinpol	1924.70		NIST Webbook
rinpol	1924.70		NIST Webbook
tb	563.74	K	Cheméo Relay (1.0)
tf	493.31	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1421494&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point