Di-tert-butyl butanedioate

Other names: butanedioic acid, 1,4-bis(1,1-dimethylethyl) ester
di-tert-butyl succinate
Inchi: InChI=1S/C12H22O4/c1-11(2,3)15-9(13)7-8-10(14)16-12(4,5)6/h7-8H2,1-6H3
InchiKey: GOORECODRBZTKF-UHFFFAOYSA-N
Formula: C12H22O4
SMILES: CC(C)(C)OC(=O)CCC(=O)OC(C)(C)C
Mol. weight [g/mol]: 230.30

Physical Properties

Property code	Value	Unit	Source
gf	-412.00	kJ/mol	Joback Method
hf	-798.11	kJ/mol	Joback Method
hfus	63.88	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	61.93	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	63.15	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	62.18	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	63.39	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	62.91	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids

hfus	63.64	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	62.42	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	61.69	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	65.59	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	65.22	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	64.61	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	64.37	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	64.12	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	62.66	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	62.91	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hvap	58.03	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.450		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	1242.00		NIST Webbook
tb	620.08	K	Joback Method
tc	815.26	K	Joback Method

tf	374.16	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.98	J/mol×K	620.08	Joback Method
cpg	537.75	J/mol×K	652.61	Joback Method
cpg	552.63	J/mol×K	685.14	Joback Method
cpg	566.64	J/mol×K	717.67	Joback Method
cpg	579.82	J/mol×K	750.20	Joback Method
cpg	592.18	J/mol×K	782.73	Joback Method
cpg	603.78	J/mol×K	815.26	Joback Method
dvisc	0.0019720	Pa×s	374.16	Joback Method
dvisc	0.0009780	Pa×s	415.15	Joback Method
dvisc	0.0005501	Pa×s	456.13	Joback Method
dvisc	0.0003403	Pa×s	497.12	Joback Method
dvisc	0.0002264	Pa×s	538.11	Joback Method
dvisc	0.0001596	Pa×s	579.09	Joback Method
dvisc	0.0001179	Pa×s	620.08	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids:	https://www.doi.org/10.1016/j.fluid.2011.07.007
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=R633022&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