Di-t-butyl malonate

Other names:	bis(1,1-dimethylethyl) malonate
	bis(1,1-dimethylethyl) propanedioate
	di-t-Butylmalonate
	di-tert-butyl malonate
	malonic acid, di-tert-butyl ester
	propanedioic acid, bis(1,1-dimethylethyl) ester
	tert-butyl malonate
Inchi:	InChI=1S/C11H20O4/c1-10(2,3)14-8(12)7-9(13)15-11(4,5)6/h7H2,1-6H3
InchiKey:	CLPHAYNBNTVRDI-UHFFFAOYSA-N
Formula:	C11H20O4
SMILES:	CC(C)(C)OC(=O)CC(=O)OC(C)(C)C
Mol. weight [g/mol]:	216.28

Physical Properties

Property code	Value	Unit	Source
hf	-949.02	kJ/mol	Cheméo Relay (1.0)
hfus	62.90	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	60.76	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	65.73	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	65.39	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	65.17	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids

hfus	64.83	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	64.60	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	64.14	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	63.80	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	63.58	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	63.35	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	63.12	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	66.29	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	66.07	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	61.77	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	62.78	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids

hfus	61.44	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	61.10	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	62.45	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	60.41	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hvap	67.23	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.35		Cheméo Relay (1.0)
logp	2.060		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
tb	484.37	K	Cheméo Relay (1.0)
tc	670.73	K	Cheméo Relay (1.0)
tf	273.33	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.37	J/mol×K	597.20	Joback Method
cpg	550.41	J/mol×K	794.92	Joback Method
cpg	539.22	J/mol×K	761.97	Joback Method
cpg	527.28	J/mol×K	729.01	Joback Method
cpg	514.56	J/mol×K	696.06	Joback Method
cpg	501.01	J/mol×K	663.11	Joback Method
cpg	486.63	J/mol×K	630.15	Joback Method
dvisc	0.0003876	Pa×s	480.05	Joback Method
dvisc	0.0001359	Pa×s	597.20	Joback Method
dvisc	0.0001836	Pa×s	558.15	Joback Method
dvisc	0.0002593	Pa×s	519.10	Joback Method
dvisc	0.0021736	Pa×s	362.89	Joback Method
dvisc	0.0006219	Pa×s	440.99	Joback Method
dvisc	0.0010941	Pa×s	401.94	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.70	K	2.90	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C541162&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

Cheméo Relay (1.0):

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point