Succinic acid diisopropyl ester

Other names:	Diisopropyl butanedioate
	bis(1-methylethyl) butanedioate
	butanedioic acid, bis(1-methylethyl) ester
	diisopropyl succinate
	succinic acid, diisopropyl ester
Inchi:	InChI=1S/C10H18O4/c1-7(2)13-9(11)5-6-10(12)14-8(3)4/h7-8H,5-6H2,1-4H3
InchiKey:	YPLYFEUBZLLLIY-UHFFFAOYSA-N
Formula:	C10H18O4
SMILES:	CC(C)OC(=O)CCC(=O)OC(C)C
Mol. weight [g/mol]:	202.25
CAS:	924-88-9

Physical Properties

Property code	Value	Unit	Source
gf	-439.40	kJ/mol	Joback Method
hf	-749.89	kJ/mol	Joback Method
hfus	65.23	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	66.63	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	66.31	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	66.08	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	65.77	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids

hfus	65.55	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	66.95	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	65.00	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	64.69	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	64.48	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	67.60	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	67.28	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hvap	55.39	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.670		Crippen Method
mcvol	166.640	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	1225.00		NIST Webbook
rinpol	1226.00		NIST Webbook
tb	579.90	K	Joback Method
tc	766.72	K	Joback Method
tf	316.78	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.45	J/mol×K	579.90	Joback Method

cpg	430.24	J/mol×K	611.04	Joback Method
cpg	443.43	J/mol×K	642.17	Joback Method
cpg	456.03	J/mol×K	673.31	Joback Method
cpg	468.03	J/mol×K	704.45	Joback Method
cpg	479.43	J/mol×K	735.58	Joback Method
cpg	490.22	J/mol×K	766.72	Joback Method
dvisc	0.0031886	Pa×s	316.78	Joback Method
dvisc	0.0014437	Pa×s	360.63	Joback Method
dvisc	0.0007762	Pa×s	404.49	Joback Method
dvisc	0.0004712	Pa×s	448.34	Joback Method
dvisc	0.0003126	Pa×s	492.19	Joback Method
dvisc	0.0002218	Pa×s	536.05	Joback Method
dvisc	0.0001658	Pa×s	579.90	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=C924889&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