PROPANEDIOIC ACID, BIS(1-METHYLETHYL) ESTER

Other names: diisopropyl malonate
dipropan-2-yl propanedioate
propanedioic acid, 1,3-bis(1-methylethyl) ester
Inchi: InChI=1S/C9H16O4/c1-6(2)12-8(10)5-9(11)13-7(3)4/h6-7H,5H2,1-4H3
InchiKey: QRVSDVDFJFKYKA-UHFFFAOYSA-N
Formula: C9H16O4
SMILES: CC(C)OC(=O)CC(=O)OC(C)C
Mol. weight [g/mol]: 188.22

Physical Properties

Property code	Value	Unit	Source
hf	-901.27	kJ/mol	Cheméo Relay (1.0)
hfus	61.60	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	61.50	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	64.81	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	64.49	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	64.20	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	63.90	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids

hfus	63.60	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	63.30	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	63.00	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	62.70	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	62.40	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	62.20	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	62.09	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	61.90	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	61.40	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	61.81	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	61.21	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hvap	65.56	kJ/mol	Cheméo Relay (1.0)
ie	9.80	eV	Cheméo Relay (1.0)
log10ws	-1.70		Cheméo Relay (1.0)
logp	1.280		Crippen Method

mcvol	152.550	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	1113.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1115.00		NIST Webbook
tb	451.84	K	Cheméo Relay (1.0)
tc	641.12	K	Cheméo Relay (1.0)
tf	234.81	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.76	J/mol×K	557.02	Joback Method
cpg	381.74	J/mol×K	588.51	Joback Method
cpg	394.19	J/mol×K	620.01	Joback Method
cpg	406.09	J/mol×K	651.50	Joback Method
cpg	417.44	J/mol×K	683.00	Joback Method
cpg	428.24	J/mol×K	714.49	Joback Method
cpg	438.48	J/mol×K	745.99	Joback Method
dvisc	0.0033834	Pa×s	305.51	Joback Method
dvisc	0.0015540	Pa×s	347.43	Joback Method
dvisc	0.0008440	Pa×s	389.35	Joback Method
dvisc	0.0005161	Pa×s	431.26	Joback Method
dvisc	0.0003443	Pa×s	473.18	Joback Method
dvisc	0.0002454	Pa×s	515.10	Joback Method
dvisc	0.0001840	Pa×s	557.02	Joback Method

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=C13195647&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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point