Glutaric acid, diisopropyl ester

Other names:	bis(1-methylethyl) pentanedioate
	diisopropyl glutarate
	pentanedioic acid, bis(1-methylethyl) ester
Inchi:	InChI=1S/C11H20O4/c1-8(2)14-10(12)6-5-7-11(13)15-9(3)4/h8-9H,5-7H2,1-4H3
InchiKey:	MSQKMFXJFBXZNQ-UHFFFAOYSA-N
Formula:	C11H20O4
SMILES:	CC(C)OC(=O)CCCC(=O)OC(C)C
Mol. weight [g/mol]:	216.28

Physical Properties

Property code	Value	Unit	Source
hf	-935.62	kJ/mol	Cheméo Relay (1.0)
hfus	70.88	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	70.17	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	71.94	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	71.59	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	71.23	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	72.98	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids

hfus	70.53	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	72.28	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	69.70	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	69.50	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	69.15	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	72.63	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hvap	66.64	kJ/mol	Cheméo Relay (1.0)
ie	9.62	eV	Cheméo Relay (1.0)
log10ws	-2.08		Cheméo Relay (1.0)
logp	2.060		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1322.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1321.00		NIST Webbook
rinpol	1323.00		NIST Webbook
tb	485.95	K	Cheméo Relay (1.0)
tc	665.28	K	Cheméo Relay (1.0)
tf	267.42	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	465.83	J/mol×K	602.78	Joback Method
cpg	480.33	J/mol×K	633.59	Joback Method
cpg	494.18	J/mol×K	664.41	Joback Method
cpg	507.38	J/mol×K	695.22	Joback Method
cpg	519.94	J/mol×K	726.03	Joback Method
cpg	531.86	J/mol×K	756.85	Joback Method
cpg	543.12	J/mol×K	787.66	Joback Method
dvisc	0.0029767	Pa×s	328.05	Joback Method
dvisc	0.0013297	Pa×s	373.84	Joback Method
dvisc	0.0007082	Pa×s	419.63	Joback Method
dvisc	0.0004269	Pa×s	465.41	Joback Method
dvisc	0.0002818	Pa×s	511.20	Joback Method
dvisc	0.0001992	Pa×s	556.99	Joback Method
dvisc	0.0001484	Pa×s	602.78	Joback Method

Sources

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=C71340460&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):	
Cheméo Relay (1.0, beta):	

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