Propanedioic acid, dipropyl ester

Other names:	1,3-propanedioic acid, dipropyl ester
	Di-n-propyl malonate
	dipropyl 1,3-propanedioate
	dipropyl malonate
	malonic acid, dipropyl ester
Inchi:	InChI=1S/C9H16O4/c1-3-5-12-8(10)7-9(11)13-6-4-2/h3-7H2,1-2H3
InchiKey:	LWIWFCDNJNZEKB-UHFFFAOYSA-N
Formula:	C9H16O4
SMILES:	CCCOC(=O)CC(=O)OCCC
Mol. weight [g/mol]:	188.22
CAS:	1117-19-7

Physical Properties

Property code	Value	Unit	Source
gf	-442.94	kJ/mol	Joback Method
hf	-718.69	kJ/mol	Joback Method
hfus	24.64	kJ/mol	Joback Method
hvap	53.94	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.283		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	1221.00		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1220.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1700.00		NIST Webbook
tb	502.40 ± 0.70	K	NIST Webbook
tc	739.72	K	Joback Method
tf	196.10 ± 1.00	K	NIST Webbook
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.00	J/mol×K	739.72	Joback Method
cpg	380.43	J/mol×K	588.20	Joback Method
cpg	392.33	J/mol×K	618.51	Joback Method
cpg	403.74	J/mol×K	648.81	Joback Method
cpg	414.66	J/mol×K	679.11	Joback Method
cpg	425.08	J/mol×K	709.42	Joback Method
cpg	368.05	J/mol×K	557.90	Joback Method
dvisc	0.0002660	Pa×s	520.84	Joback Method
dvisc	0.0003515	Pa×s	483.77	Joback Method
dvisc	0.0004864	Pa×s	446.70	Joback Method
dvisc	0.0007139	Pa×s	409.64	Joback Method
dvisc	0.0011310	Pa×s	372.57	Joback Method
dvisc	0.0002089	Pa×s	557.90	Joback Method
dvisc	0.0019834	Pa×s	335.51	Joback Method
pvap	0.02	kPa	313.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.02	kPa	311.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.03	kPa	318.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.03	kPa	319.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids

pvap	0.04	kPa	323.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.06	kPa	328.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.09	kPa	333.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.11	kPa	336.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.13	kPa	338.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.01	kPa	308.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.01	kPa	307.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	

pvap	8.97e-03	kPa	303.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	6.52e-03	kPa	299.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	5.82e-03	kPa	298.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	3.56e-03	kPa	293.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.02	kPa	315.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids:	https://www.doi.org/10.1021/je100231g
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=C1117197&Units=SI

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume