Propanedioic acid, methyl-, diethyl ester

Other names:	Diethyl 2-methylmalonate
	Ethyl methylmalonate
	Malonic acid, methyl-, diethyl ester
	Methylmalonic acid diethyl ester
	Propanedioic acid, 2-methyl-, diethyl ester
	diethyl isosuccinate
	diethyl methylmalonate
	diethyl methylpropanedioate
Inchi:	InChI=1S/C8H14O4/c1-4-11-7(9)6(3)8(10)12-5-2/h6H,4-5H2,1-3H3
InchiKey:	UPQZOUHVTJNGFK-UHFFFAOYSA-N
Formula:	C8H14O4
SMILES:	CCOC(=O)C(C)C(=O)OCC
Mol. weight [g/mol]:	174.19
CAS:	609-08-5

Physical Properties

Property code	Value	Unit	Source
gf	-453.80	kJ/mol	Joback Method
hf	-703.33	kJ/mol	Joback Method
hfus	18.53	kJ/mol	Joback Method
hvap	51.33	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	0.749		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rinpol	1073.00		NIST Webbook
rinpol	1073.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1539.00		NIST Webbook
tb	474.20	K	NIST Webbook
tb	471.70	K	NIST Webbook
tc	722.01	K	Joback Method
tf	309.24	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.20	J/mol×K	722.01	Joback Method
cpg	334.30	J/mol×K	565.82	Joback Method
cpg	345.61	J/mol×K	597.06	Joback Method
cpg	356.46	J/mol×K	628.29	Joback Method
cpg	366.85	J/mol×K	659.53	Joback Method
cpg	376.76	J/mol×K	690.77	Joback Method
cpg	322.54	J/mol×K	534.58	Joback Method
dvisc	0.0002792	Pa×s	497.02	Joback Method
dvisc	0.0003777	Pa×s	459.47	Joback Method
dvisc	0.0005393	Pa×s	421.91	Joback Method
dvisc	0.0008255	Pa×s	384.35	Joback Method
dvisc	0.0013856	Pa×s	346.80	Joback Method
dvisc	0.0002153	Pa×s	534.58	Joback Method
dvisc	0.0026376	Pa×s	309.24	Joback Method
hvapt	52.50	kJ/mol	393.50	NIST Webbook
pvap	34.43	kPa	433.15	Vapor Pressures of Morpholine, Diethyl Methylmalonate, and Five Glycol Ethers at Temperatures up to 473.15 K
pvap	62.44	kPa	453.15	Vapor Pressures of Morpholine, Diethyl Methylmalonate, and Five Glycol Ethers at Temperatures up to 473.15 K
pvap	71.52	kPa	458.15	Vapor Pressures of Morpholine, Diethyl Methylmalonate, and Five Glycol Ethers at Temperatures up to 473.15 K
pvap	81.75	kPa	463.15	Vapor Pressures of Morpholine, Diethyl Methylmalonate, and Five Glycol Ethers at Temperatures up to 473.15 K

pvap	92.85	kPa	468.15	Vapor Pressures of Morpholine, Diethyl Methylmalonate, and Five Glycol Ethers at Temperatures up to 473.15 K	
pvap	17.40	kPa	413.15	Vapor Pressures of Morpholine, Diethyl Methylmalonate, and Five Glycol Ethers at Temperatures up to 473.15 K	
pvap	11.84	kPa	403.15	Vapor Pressures of Morpholine, Diethyl Methylmalonate, and Five Glycol Ethers at Temperatures up to 473.15 K	
pvap	7.94	kPa	393.15	Vapor Pressures of Morpholine, Diethyl Methylmalonate, and Five Glycol Ethers at Temperatures up to 473.15 K	
pvap	5.02	kPa	383.15	Vapor Pressures of Morpholine, Diethyl Methylmalonate, and Five Glycol Ethers at Temperatures up to 473.15 K	
pvap	3.15	kPa	373.15	Vapor Pressures of Morpholine, Diethyl Methylmalonate, and Five Glycol Ethers at Temperatures up to 473.15 K	
pvap	46.74	kPa	443.15	Vapor Pressures of Morpholine, Diethyl Methylmalonate, and Five Glycol Ethers at Temperatures up to 473.15 K	

pvap	24.82	kPa	423.15	Vapor Pressures of Morpholine, Diethyl Methylmalonate, and Five Glycol Ethers at Temperatures up to 473.15 K

Sources

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=C609085&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressures of Morpholine, Diethyl Methylmalonate, and Five Glycol Ethers at Temperatures up to 473.15 K:	https://www.doi.org/10.1021/je049627d

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
hvapt:	Enthalpy of vaporization at a given temperature
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