Diethyl tert-butylmalonate

Other names:	Diethyl t-butylmalonate
	Propanedioic acid, (1,1-dimethylethyl)-, diethyl ester
	diethyl (1,1-dimethylethyl)malonate
Inchi:	InChI=1S/C11H20O4/c1-6-14-9(12)8(11(3,4)5)10(13)15-7-2/h8H,6-7H2,1-5H3
InchiKey:	RJNICNBRGVKNSR-UHFFFAOYSA-N
Formula:	C11H20O4
SMILES:	CCOC(=O)C(C(=O)OCC)C(C)(C)C
Mol. weight [g/mol]:	216.27
CAS:	759-24-0

Physical Properties

Property code	Value	Unit	Source
gf	-425.70	kJ/mol	Joback Method
hf	-774.00	kJ/mol	Joback Method
hfus	18.88	kJ/mol	Joback Method
hvap	56.71	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.775		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
tb	599.99	K	Joback Method
tc	791.04	K	Joback Method
tf	345.47	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.59	J/mol×K	599.99	Joback Method
cpg	483.45	J/mol×K	631.83	Joback Method
cpg	497.56	J/mol×K	663.67	Joback Method
cpg	510.92	J/mol×K	695.51	Joback Method
cpg	523.56	J/mol×K	727.36	Joback Method
cpg	535.49	J/mol×K	759.20	Joback Method

cpg	546.72	J/mol×K	791.04	Joback Method
dvisc	0.0025750	Pa×s	345.47	Joback Method
dvisc	0.0012195	Pa×s	387.89	Joback Method
dvisc	0.0006692	Pa×s	430.31	Joback Method
dvisc	0.0004090	Pa×s	472.73	Joback Method
dvisc	0.0002711	Pa×s	515.15	Joback Method
dvisc	0.0001913	Pa×s	557.57	Joback Method
dvisc	0.0001418	Pa×s	599.99	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.20	K	1.50	NIST Webbook

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=C759240&Units=SI
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
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
tb: Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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