Diethyl sec-butylmalonate

Other names:	Diethyl 1-methylpropylmalonate
	Diethyl s-butylmalonate
	sec-Butylmalonic acid diethyl ester
	Propanedioic acid, (1-methylpropyl)-, diethyl ester
	Malonic acid, sec-butyl-, diethyl ester
Inchi:	InChI=1S/C11H20O4/c1-5-8(4)9(10(12)14-6-2)11(13)15-7-3/h8-9H,5-7H2,1-4H3
InchiKey:	MIIZSUOEOUHAIZ-UHFFFAOYSA-N
Formula:	C11H20O4
SMILES:	CCOC(=O)C(C(=O)OCC)C(C)CC
Mol. weight [g/mol]:	216.27
CAS:	83-27-2

Physical Properties

Property code	Value	Unit	Source
gf	-430.98	kJ/mol	Joback Method
hf	-770.53	kJ/mol	Joback Method
hfus	22.77	kJ/mol	Joback Method
hvap	57.62	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.775		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
tb	602.78	K	Joback Method
tc	787.66	K	Joback Method
tf	328.05	K	Joback Method
vc	0.688	m3/kmol	Joback Method

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.00 ± 2.00	K	2.40	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C83272&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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