Propanedioic acid, (1-methylethylidene)-, diethyl ester

Other names: Malonic acid, isopropylidene-, diethyl ester
Propanedioic acid, (1-methylethylidene)-, diethyl ester
Inchi: InChI=1S/C10H16O4/c1-5-13-9(11)8(7(3)4)10(12)14-6-2/h5-6H2,1-4H3
InchiKey: WEISAZNMMVPNTH-UHFFFAOYSA-N
Formula: C10H16O4
SMILES: CCOC(=O)C(C(=O)OCC)=C(C)C
Mol. weight [g/mol]: 200.23

Physical Properties

Property code	Value	Unit	Source
af	0.6102		Cheméo Relay (1.0)
gf	-371.40	kJ/mol	Joback Method
hf	-758.84	kJ/mol	Cheméo Relay (1.0)
hfus	24.81	kJ/mol	Joback Method
hvap	63.67	kJ/mol	Cheméo Relay (1.0)
ie	8.94	eV	Cheméo Relay (1.0)
log10ws	-2.34		Cheméo Relay (1.0)
logp	1.449		Crippen Method
mcvol	162.340	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
tb	517.52	K	Cheméo Relay (1.0)
tc	683.93	K	Cheméo Relay (1.0)
tf	245.88	K	Cheméo Relay (1.0)
vc	0.607	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.45	J/mol×K	584.70	Joback Method
cpg	408.51	J/mol×K	616.90	Joback Method
cpg	420.96	J/mol×K	649.10	Joback Method
cpg	432.81	J/mol×K	681.31	Joback Method
cpg	444.07	J/mol×K	713.51	Joback Method
cpg	454.74	J/mol×K	745.71	Joback Method

cpg	464.83	J/mol×K	777.91	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	449.70	K	16.00	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6802751&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):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
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
ie: Ionization energy
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