

Diethyl isopropylidenemalonate

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
CAS:	6802-75-1

Physical Properties

Property code	Value	Unit	Source
gf	-371.40	kJ/mol	Joback Method
hf	-641.69	kJ/mol	Joback Method
hfus	24.81	kJ/mol	Joback Method
hvap	56.28	kJ/mol	Joback Method
log10ws	-1.59		Crippen Method
logp	1.449		Crippen Method
mcvol	162.340	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
tb	584.70	K	Joback Method
tc	777.91	K	Joback Method
tf	313.78	K	Joback Method
vc	0.625	m3/kmol	Joback Method

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

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=C6802751&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
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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