

Diethyl methyl-isopropylmalonate

Other names:	Diethyl isopropylmethylmalonate
Inchi:	InChI=1S/C11H20O4/c1-6-14-9(12)11(5,8(3)4)10(13)15-7-2/h8H,6-7H2,1-5H3
InchiKey:	NQSVPQIOJRYMGQ-UHFFFAOYSA-N
Formula:	C11H20O4
SMILES:	CCOC(=O)C(C)(C(=O)OCC)C(C)C
Mol. weight [g/mol]:	216.27
CAS:	58447-69-1

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/molxK	599.99	Joback Method
cpg	483.45	J/molxK	631.83	Joback Method
cpg	497.56	J/molxK	663.67	Joback Method
cpg	510.92	J/molxK	695.51	Joback Method
cpg	523.56	J/molxK	727.36	Joback Method
cpg	535.49	J/molxK	759.20	Joback Method
cpg	546.72	J/molxK	791.04	Joback Method
dvisc	0.0025750	Paxs	345.47	Joback Method

dvisc	0.0012195	Paxs	387.89	Joback Method
dvisc	0.0006692	Paxs	430.31	Joback Method
dvisc	0.0004090	Paxs	472.73	Joback Method
dvisc	0.0002711	Paxs	515.15	Joback Method
dvisc	0.0001913	Paxs	557.57	Joback Method
dvisc	0.0001418	Paxs	599.99	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C58447691&Units=SI

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/92-747-1/Diethyl-methyl-isopropylmalonate.pdf>

Generated by Cheméo on 2024-04-26 08:06:37.932742493 +0000 UTC m=+16408046.853319804.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.